AD-A080 415 AIR FORCE INST OF TECH WRIGHT-PATTERSON AFB OH SCHOO--ETC F/G 12/1
NUMERICAL METHODS AND THE SOLUTION OF BOUNDARY VALUE PROBLEMS.(U)
DEC 79 G N NELSON
UNCLASSIFIED AFIT/GEP/PH/79D-7 NL

1 OF 2
AD
A080415

LEVEL II

ADA080415

DDC
RECEIVED
FEB 8 1980
A

DDC FILE COPY

UNITED STATES AIR FORCE

AIR UNIVERSITY

AIR FORCE INSTITUTE OF TECHNOLOGY

Wright-Patterson Air Force Base, Ohio

DISTRIBUTION STATEMENT A
Approved for public release;
Distribution Unlimited

80 2 5 243

AFIT/GEP/PH/79D-7

6 NUMERICAL METHODS AND THE SOLUTION OF BOUNDARY VALUE PROBLEMS.

9 Master's THESIS,

14 AFIT/GEP/PH/79D-7

10 Gale N. Nelson
Capt. USAF

11 Dec 79

12 157

Approved for public release; distribution unlimited

012225

mt

AFIT/GEP/PH/79D-7

NUMERICAL METHODS AND THE SOLUTION OF BOUNDARY VALUE PROBLEMS

THESIS

Presented to the Faculty of the School of Engineering
of the Air Force Institute of Technology
Air University
in Partial Fulfillment of the
Requirements for the Degree of
Master of Science

by

Gale N. Nelson, B.S.
Capt. USAF
Graduate Engineering Physics

December 1979

Approved for public release; distribution unlimited

Preface

This report is the result of my investigation into numerical solutions of differential equations, expressed in both differential and integral form. The method of finite differences was utilized for solutions of the equations in differential form. A Fredholm integral representation was developed and numerically evaluated to compare with the finite difference method. The purpose of this thesis was to examine the solutions obtained to the differential equation using both above methods and report on the advantages and disadvantages of each. A secondary purpose of this thesis was to strengthen my own mathematical background on numerical methods and their ability to solve differential equations. I have attempted to include sufficient detail to provide the reader with a step by step account of the development.

I want to thank Dr. Bernard Kaplan, my advisor, for his guidance and assistance throughout this study. I would also like to thank Dr. John Jones for his many helpful discussions pertaining to spline theory and also to Dr. Wilhelm Ericksen for his patience in helping correct many of my computer programs. I also wish to thank Dr. W. Kessler of the Air Force Materials Laboratory for sponsoring this study. Finally, I

would like to thank my wife, Carolyn, for her patience, understanding and typing.

Contents

	Page
Preface	ii
List of Figures	vii
List of Tables	ix
Abstract	x
I. Introduction	1
Background	1
Numerical Techniques	1
One-Dimensional Cases	2
Two-Dimensional Cases	3
Purpose	3
Plan of Development	4
II. Theory	6
Integral Equations	6
Multiple Integrations	7
Differential Conversion to Integral Form	7
Kernel Properties	10
The Green's Function	11
Determining the Green's Function	12
Example	14
The Green's Integral Equation	17
Equivalency of the Integral Equation and the Green's Integral	20
Integral Representation	22
Numerical Integration	24
Trapezoid Rule	25
Trapezoid vs. Simpson's Rule	26
Finite Difference Method	30
Matrix Methods: The Integral Form of Solution	33
Matrix Methods: The Method of Finite Differences	35
Simultaneous Solution of Linear Equations	38

Page

III. One-Dimensional Problems..... 44

Computer Programs..... 44
LEQT1F - IMSL Subroutine..... 45
Case I..... 45
Analytical Solution..... 46
Integral Solution..... 47
Finite Differences..... 50
First Forward Difference..... 52
Error Analysis..... 53
Simpson's Comparison..... 56
Times of Solution..... 61
Accuracy..... 62
Conclusions..... 64
Case II..... 65
Analytical Solution..... 65
Integral Solution..... 66
Green's Integral..... 69
Finite Differences..... 70
Relative Error..... 72
Error Analysis..... 72
Times of Solution..... 79
Conclusions..... 79
Case III..... 80
Analytical Solution..... 81
Integral Solution..... 81
Green's Integral..... 85
Finite Differences..... 86
Relative Error..... 88
Error Analysis..... 88
Simpson's Comparison..... 95
Times of Solution..... 98
Conclusions..... 98

IV. Two-Dimensional Numerical Methods..... 100

The Steady-State
Heat Conduction Problem..... 100
Analytical Solution..... 101
Finite Differences..... 102
81 Interior Nodes..... 104
Results..... 105
Comments - Finite Differences..... 106
Introduction - Splines..... 108
Spline Functions..... 109

Page

Integral Method of Solution..... 111
Spline Integration..... 112
Results..... 113
Conclusions..... 114

V. Conclusions and Recommendations..... 116

Conclusions: One-Dimensional Cases... 116
Conclusions: Two-Dimensional Cases... 117
Recommendations..... 118

Bibliography..... 119

Appendix A: Kernel Properties of the Equation $\frac{d^2y}{dx^2} + A\frac{dy}{dx} + By = 0$ for $A \neq 0$ 121

Appendix B: Determining the Green's Function for the One-Dimensional Helmholtz Equation..... 124

Appendix C: Determining the Green's Function for Case III..... 127

Appendix D: Analytical Solution for the Two-Dimensional Steady-State Heat Conduction Problem..... 131

Appendix E: Derivation of the Cubic Spline Function..... 136

Appendix F: Integration, Using the Cubic Spline Function..... 139

Vita..... 142

List of Figures

Figure		Page
1	The Integral Kernel, $K(x,\xi)$	11
2	Trapezoid Partition.....	25
3	The Linear Kernel, $K(x,\xi)$	27
4	Quadratic Interpolation Across the Discontinuity, $\xi = 2/3$	29
5	Flow Diagram for Computer Programs Using Numerical Integration/Differentiation.	44
6	Analytic Solution, Case I.....	48
7	Comparison of Relative Errors.....	54
8	Relative Errors Using Simpson's Rule.....	58
9	Relative Errors Using Trapezoid Rule.....	59
10	Analytic Solution, Case II.....	67
11	Comparison of Relative Errors.....	73
12	Relative Errors of Array Elements Integral - CFD methods.....	76
13	Relative Errors of Array Elements Green's Integral Equation.....	77
14	Analytic Solution, Case III.....	82
15	Comparison of Relative Errors.....	89
16	Relative Errors of Array Elements Integral Equation Method.....	93
17	Relative Errors of Array Elements CFD Method.....	94
18	Relative Errors Using Trapezoid Rule.....	96
19	Relative Errors Using Simpson's Rule.....	97
20	Two-Dimensional Steady-State Heat Conduction Problem.....	100

Figure		Page
21	Interior Grid Network.....	102
22	Interior Nodal Arrangement.....	103
23	Finite Difference Scheme Using Three Points Parallel to the X-Axis.....	106
24	Finite Difference Scheme Using Three Points Parallel to the Y-Axis.....	107
25	Method of Harmonic Solutions for the Poisson Equation.....	132
26	Derivative of Cubic Spline Function, $S_k(x)$....	137

List of Tables

Table		Page
I	Relative Error (%) - Computer Solutions for $y''+y=0$, $x=.5$	53
II	Error Trends Using Trapezoid Rule	57
III	Error Trends Using Finite Difference Methods for $y''+y=0$, $x=.5$	61
IV	Computer Time - $y''+y=0$	61
V	Relative Error (%) - Computer Solutions for $y''+\lambda^2 y=1$, $x=.5$	72
VI	Error Trends - Computer Solutions for $y''+\lambda^2 y=1$, $x=.5$	75
VII	Computer Time - $y''+\lambda^2 y=1$	79
VIII	Relative Error (%) - Computer Solutions for $x^2y''-2y=x^4$, $x=2$	88
IX	Error Trends - Computer Solutions for $x^2y''-2y=x^4$, $x=2$	91
X	Computer Time - $x^2y''-2y=x^4$	98
XI	Finite Difference Solution for Square, with Heat Generation	105
XII	Cubic Spline Solution for Square, with Heat Generation	114

Abstract

A study of several numerical methods for the solution of boundary value problems, in both one and two-dimensions, was conducted using the CDC 6600 computer. The method of finite differences was employed for solution of the equations in differential form. These numerical solutions were compared to those obtained by transforming the original differential equation into integral form and approximating their solution using numerical integration via the trapezoid rule. All numerical experiments were conducted using Dirichlet boundary conditions.

In the one-dimensional cases studied it was found that both methods are equivalent, i.e., yield identical solutions when the integral representation had a linear weighted Green's function kernel. In addition, the integral approach was found to be as accurate in all one-dimensional cases as the method of finite differences. The finite difference method proved quicker than the numerical integration techniques in all but one test case where the Green's integral representation was examined.

For the two-dimensional investigation the steady-state heat conduction equation was analyzed. Again, the method of finite differences in two-dimensions next page

cont. was compared to the integral approach, using cubic splines. The method of finite differences was found to be superior in calculating the internal temperature, at all nodal points, as compared to the integral-spline solution.

I. Introduction

Background

A majority of problems encountered in technical research by engineers and physicists can be expressed in mathematical form as a differential or partial differential equation. Solutions of these equations are dependent upon initial conditions and/or boundary values. (If the values of the function are specified on the boundary, the equation is said to contain Dirichlet boundary conditions. If the normal derivatives (gradients) of the function are specified on the boundary then Neumann boundary conditions are said to exist. The boundary conditions are referred to as mixed if the initial conditions describing the differential or partial differential equation contain both Dirichlet and Neumann conditions.) Because the equations possess unique solutions it does not necessarily follow that these solutions are easy to obtain. In many cases the exact closed-form solutions are not attainable; and as a result, approximation techniques must be used to generate analytical values. For this reason, most of all important problems require application of some numerical method.

Numerical Techniques

Though there are a variety of techniques available

to handle specific boundary value problems, this thesis will be concerned with three specific methods:

(1) The method of finite differences

(2) Fredholm integral equations and their numerical approximations

(3) Utilization of cubic splines

One-Dimensional Cases

The method of finite differences is based upon a scheme of numerical differentiation. The original differential equation is replaced by a finite number of algebraic expressions defined over the interval; this set of equations is easily solved using the computer. In the one-dimensional cases methods (1) and (2) are compared for both accuracy and speed of computations.

The second method transforms the original differential expression into an equivalent integral equation, usually a Fredholm integral equation of the second or third kind (Ref 1: 381-382). The advantages of this technique is that in many cases a weighted symmetric Green's function kernel results and can be evaluated using standard numerical integration techniques, such as the trapezoid rule.

Two-Dimensional Cases

In the two-dimensional analysis the steady-state heat conduction problem, with an inhomogeneous boundary condition of T_0 along one edge, was investigated. The analytical solution was calculated and compared at 16 interior nodal points with the method of finite differences.

The third method investigated in the two-dimensional case was again one of converting the original partial differential equation into integral form by a method proposed by Hajdin and Krajcinovic (Ref 2: 523-539). The unknowns appearing within the integrals are approximated by cubic splines and numerically integrated. Again methods (1) and (3) were compared for both accuracy and ease of computation.

Purpose

There are several important for investigating numerical integration techniques two methods bases upon numerical differentiation. Computer utilization costs are normally are direct function of utilization time. Thus it becomes of prime importance to use the most cost effective method in solving a particular problem. Hajdin and Krajcinovic contend that numerical integration is many times more accurate than numerical differentiation and that results through numerical

integration should be superior to those based upon the method of finite differences. For the same accuracy one should be able to significantly reduce the number of points (i.e. number of algebraic equations) with numerical integration (Ref 3: 509-510). The purpose of this study is therefore to determine whether or not numerical integration is advantageous or comparable to the method of finite differences, a method of numerical differentiation.

Plan of Development

Due to time restrictions placed on this study, four types of problems were considered. In the one-dimensional analysis the problems and boundary conditions were the following:

$$\left.\begin{array}{ll} (1)\ y'' + y = 0, & y(0) = 0,\ y(1) = 1 \\ (2)\ y'' + \lambda^2 y = 1, & y(0) = 0,\ y(1) = 0 \\ (3)\ x^2 y'' - 2y = x^4, & y(1) = 0,\ y(3) = 0 \end{array}\right\} \quad (1)$$

Equation (1), equivalent to the one-dimensional Helmholtz equation, is introduced to illustrate the procedures used in transforming differential equations into their equivalent integral representation. In addition, equation (1) is also used to demonstrate the numerical methods employed to evaluate the Fredholm integral representations of equations (2) and (3).

All equations had closed-form analytical solutions that were used for comparison to the numerically generated values. Numerical computation was carried out on the CDC 6600 computer using identical numerical techniques in all cases. Also, the number of iterations per interval was kept the same so that an accurate comparison of both methods could be made. Solutions were first obtained for 1-10 iterations over the boundary, and increased to 50 iterations/interval for the final analysis. All computation was carried to six significant decimal places.

In two-dimensional analysis, Poisson's equation was investigated. The problem chosen was the steady-state heat conduction over a square plate with an inhomogeneous Dirichlet boundary condition at one edge. The known analytical solutions were developed using the method of separation of variables. Over 10,000 independent series summations were required at each interior node point to yield six decimal place convergence. The method of finite differences was compared with the analytical results at 16 and 81 interior points. For integral conversion, the method of cubic splines was used and numerically integrated. The calculated solution was compared with the known analytic solution.

II. Theory

Integral Equations

An integral equation is one in which the function to be determined appears under an integral sign. Linear integral equations, that is, equations in which the unknown function f appears to no higher power than one, are conventionally divided into two classifications. An equation of the form

$$\alpha(x)f(x) = F(x) + \lambda\int_a^b K(x,\xi)f(\xi)\,d\xi \tag{2}$$

where α, F, and K are given functions and λ, a, and b are constants is known as a Fredholm equation. The function $K(x,\xi)$ is known as the kernel of the integral equation and is frequently a weighted Green's function. If the upper limit of the integral is not a constant the equation takes the form

$$\alpha(x)f(x) = F(x) + \lambda\int_a^x K(x,\xi)f(\xi)\,d\xi \tag{3}$$

and is known as a Volterra equation.

When $\alpha \neq 0$, equation (2) involves the unknown function f both inside and outside the integral. If $\alpha = 0$, the unknown function appears only under the integral and the equation is known as an integral equation of the first kind. If $\alpha = 1$ the equation is said to be of the second kind. In the more general case when $\alpha(x)$ is not a constant the equation is

called an integral equation of the third kind (Ref 1: 382).

Multiple Integrations

Certain integral equations can be deduced from or reduced to differential equations. In order to accomplish the reduction it is frequently necessary to make use of the formula:

$$\int_a^x\int_a^x f(x)\,dx\,dx = \int_a^x dx \int_a^\xi f(\eta)\,d\eta = \int_a^x (x-\xi) f(\xi)\,d\xi \tag{4}$$

Equation (4) is obtained by integrating the left-hand side by parts, that is

$$\left[\xi\int_a^\xi f(\eta)\,d\eta\right]_{\xi=a}^{\xi=x} - \int_a^x \xi\left\{\frac{d}{d\xi}\int_a^\xi f(\eta)\,d\eta\right\}d\xi = x\int_a^x f(\eta)\,d\eta - \int_a^x \xi f(\xi)\,d\xi \tag{5}$$

More generally, by a repeated application of this procedure, the results of integrating $f(x)$ n times over the same limits is

$$\overbrace{\int_a^x \cdots \int_a^x}^{n\text{ times}} f(x)\,\overbrace{dx \cdots dx}^{n\text{ times}} = \frac{1}{(n-1)!}\int_a^x (x-\xi)^{n-1} f(\xi)\,d\xi \tag{6}$$

Expression (6) will be useful in manipulating multiple integrations in the work which follows (Ref 4: 722).

Differential Conversion to Integral Form

To illustrate the mechanics for converting a differential equation into integral form, consider

the boundary value problem

$$\frac{d^2y}{dx^2} = -f(x) \tag{7}$$

with boundary conditions

$$y(0) = a, \qquad y(\ell) = b \tag{8}$$

First integrate both sides of (7) with respect to x over the interval $(0,x)$

$$\int_0^x \frac{d}{dx}\left(\frac{dy}{dx}\right) dx = -\int_0^x f(x)\,dx \tag{9}$$

or

$$\left.\frac{dy}{dx}\right|_0^x = -\int_0^x f(x)\,dx \tag{10}$$

Therefore (7) is equivalent to the expression

$$\frac{dy(x)}{dx} = C - \int_0^x f(x)\,dx \tag{11}$$

where C represents the unknown value of $\frac{dy(0)}{dx}$.

A second integration over $(0,x)$ leads to

$$\int_0^x \frac{d}{dx}(y)\,dx = C\int_0^x dx - \int_0^x\int_0^x f(x)\,dx\,dx \tag{12}$$

or

$$\int_0^x dy = Cx - \int_0^x\int_0^x f(x)\,dx\,dx \tag{13}$$

This becomes

$$\left.y(x)\right|_0^x = Cx - \int_0^x\int_0^x f(x)\,dx\,dx \tag{14}$$

Using equation (6) for the right-hand integral and

simplifying, equation (14) becomes

$$y(x) = y(0) + Cx - \int_0^x (x-\xi) f(\xi)\, d\xi \tag{15}$$

or

$$y(x) = a + Cx - \int_0^x (x-\xi) f(\xi)\, d\xi \tag{16}$$

The constant C can be evaluated by applying the second boundary condition, namely

$$y(\ell) = b = a + C\ell - \int_0^\ell (\ell-\xi) f(\xi)\, d\xi \tag{17}$$

Solving for C gives

$$C = \frac{b-a}{\ell} + \frac{1}{\ell}\int_0^\ell (\ell-\xi) f(\xi)\, d\xi \tag{18}$$

Substituting C above, equation (16) becomes

$$y(x) = a + \left(\frac{b-a}{\ell}\right)x + \frac{x}{\ell}\int_0^\ell (\ell-\xi) f(\xi)\, d\xi - \int_0^x (x-\xi) f(\xi)\, d\xi \tag{19}$$

This last expression can be rewritten by expanding the first integral, i.e., $\int_0^\ell = \int_0^x + \int_x^\ell$. Equation (19) then becomes

$$y(x) = a + \left(\frac{b-a}{\ell}\right)x + \frac{x}{\ell}\int_0^x (\ell-\xi) f(\xi)\, d\xi$$

$$- \int_0^x (x-\xi) f(\xi)\, d\xi + \frac{x}{\ell}\int_x^\ell (\ell-\xi) f(\xi)\, d\xi \tag{20}$$

Collecting terms under the same integral limits, (20) becomes

$$y(x) = \int_0^x \frac{\xi}{\ell}(\ell - x) f(\xi)\, d\xi + \int_x^\ell \frac{x}{\ell}(\ell - \xi) f(\xi)\, d\xi + \left(\frac{b-a}{\ell}\right) x + a \tag{21}$$

With the abbreviation

$$K(x,\xi) = \begin{cases} \frac{x}{\ell}(\ell - \xi) & x < \xi \\ \frac{\xi}{\ell}(\ell - x) & x > \xi \end{cases} \tag{22}$$

equation (21) becomes

$$y(x) = \int_0^\ell K(x,\xi) f(\xi)\, d\xi + \left(\frac{b-a}{\ell}\right) x + a \tag{23}$$

Thus, the integral equation corresponding to the boundary value problem (7) is a Fredholm equation of the second kind.

Kernel Properties

Note that the kernel, $K(x,\xi)$ given by equation (22), has different analytical expressions in the two regions, $x < \xi$ and $x > \xi$, but that the expressions are equivalent when $x = \xi$. Observe also that in each region K is a linear function of x and that K vanishes at the end points. $K(x,\xi)$ can be thought of as a function of x for a fixed value of ξ.

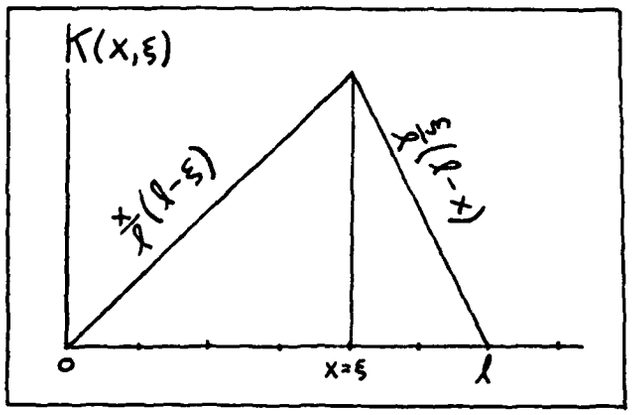

Fig. 1 The Integral Kernel, $K(x,\xi)$

Finally, $K(x,\xi)$ is unchanged if x and ξ are interchanged; that is, $K(x,\xi) = K(\xi,x)$. Kernels having this last property are said to be symmetric and obey the Reciprocity principle. Many of the kernels generated in converting boundary value problems into integral equations have this property and are commonly identified as Green's functions.

<u>The Green's Function</u>

Green's functions are extremely important mathematical quantities in physics. Mathematically, they allow the solution of differential equations to be expressed in integral form. The solution of some inhomogeneous differential equation

$$L\,y(x) + f(x) = 0 \tag{24}$$

with homogeneous boundary conditions

$$y(0) = 0, \qquad y(\ell) = 0 \tag{25}$$

and where L is the self-adjoint differential operator,

$$L = \frac{d}{dx}\left(p(x)\frac{d}{dx}\right) + q(x) \tag{26}$$

can be expressed in the integral form

$$y(x) = \int_0^{\ell} G(x,\xi) f(\xi)\, d\xi \tag{27}$$

where $G(x,\xi)$ is called the Green's function (Ref 6: 599-600). The advantages of the Green's function are:

(1) The homogeneous boundary conditions are incorporated in the integral representation (27).

(2) Equation (27) enables the differential representation, (24), to be solved via the integrating process.

(3) The Green's function method also allows solutions of (24) with inhomogeneous boundary conditions (Ref 5: 12-14).

Determining the Green's Function

The Green's function satisfies the differential operator of a homogeneous boundary value problem, everywhere except at one point. In addition, it

vanishes at the end points and has a discontinuous first derivative at $x = \xi$. For a boundary value problem of the form

$$L\, y(x) = -f(x) \tag{28}$$

the Green's function, $G(x,\xi)$, is defined as the solution of the equation

$$L\, G(x,\xi) = -\delta(x-\xi) \tag{29}$$

where $\delta(x-\xi)$ is known as the Dirac delta function having the properties

$$\delta(x-\xi) = \begin{cases} 0 & x \neq \xi \\ \infty & x = \xi \end{cases} \tag{30}$$

The Green's function satisfies the homogeneous differential operator, L , at all other points other than $x = \xi$. At $x=\xi$ a singularity exists and is governed by the properties of the delta function (Ref 15: 7). Over the interval $(0,\ell)$ it is possible to obtain a convenient form of a solution for $G(x,\xi)$ by assuming that the Green's function can be represented by $G_1(x)$ when $x<\xi$, and by $G_2(x)$ when $x>\xi$. In the one-dimensional case the Green's function has the following properties:

(1) $G(x,\xi) = \begin{cases} G_1(x) & x < \xi \\ G_2(x) & x > \xi \end{cases}$, and the functions $G_1(x)$ and $G_2(x)$ each satisfy equation (29) in their intervals of definition, i.e.,

$$L\,G_1(x) = 0, \text{ and } L\,G_2(x) = 0 \quad (\text{for } x \neq \xi) \tag{31}$$

(2) The function $G(x,\xi)$ satisfies homogeneous conditions at the interval end points $x = 0$ and $x = \ell$.

$$G_1(0) = 0, \qquad G_2(\ell) = 0 \tag{32}$$

(3) $G(x,\xi)$ is continuous at $x = \xi$. This requires that

$$G_1(\xi) = G_2(\xi) \tag{33}$$

(4) The derivative of $G(x,\xi)$ has a discontinuity of magnitude $-1/p(\xi)$ at $x = \xi$, that is,

$$\left.\frac{dG_2(x)}{dx}\right|_{x\to\xi} - \left.\frac{dG_1(x)}{dx}\right|_{x\to\xi} = -1/p(\xi) \tag{34}$$

Using these four conditions, it is possible to determine $G(x,\xi)$ and represent the solution of the differential equation in integral form.

<u>Example</u>

As an example of determining the Green's function for a differential operator, consider the boundary value problem

$$\frac{d^2y}{dx^2} = -f(x) \tag{35}$$

with inhomogeneous boundary conditions

$$y(0) = a, \qquad y(\ell) = b \tag{36}$$

The Green's function is determined as the solution of

$$L\,G(x,\xi) = -\delta(x-\xi) \tag{37}$$

where $L = \frac{d^2}{dx^2}$ in this case. Equation (37) becomes

$$\frac{d^2G(x,\xi)}{dx^2} = -\delta(x-\xi) \tag{38}$$

Assuming that $G(x,\xi)$ can be expressed by $G_1(x)$ and $G_2(x)$ over the interval $(0,\ell)$, the Green's function will be of the form

$$G(x,\xi) = \begin{cases} G_1(x) & x < \xi \\ G_2(x) & x > \xi \end{cases} \tag{39}$$

For $x \neq \xi$, $G_1(x)$ and $G_2(x)$ satisfy the homogeneous equation (31):

$$L\,G_1(x) = L\,G_2(x) = 0 \tag{40}$$

The simplest form of solution, satisfying equation (40), is to assume that $G(x,\xi)$ takes the form

$$G(x,\xi) = \begin{cases} Ax + B & x < \xi \\ Cx + D & x > \xi \end{cases} \tag{41}$$

From the previous properties (2), (3) and (4) for the Green's function, all of the constants in (41) can be evaluated. From property (2), $G(x,\xi)$ must vanish at the ends, therefore

$$G_1(0) = 0 = B \tag{42}$$

and

$$G_2(\ell) = 0 = C\ell + D, \quad \therefore D = -C\ell \tag{43}$$

Substituting these values for B and D back into (41) the Green's function becomes

$$G(x,\xi) = \begin{cases} Ax & x < \xi \\ C(x-\ell) & x > \xi \end{cases} \tag{44}$$

Using the fact that $G(x,\xi)$ is continuous at $x = \xi$, property (3), namely

$$G_1(\xi) = G_2(\xi) \tag{45}$$

the constant C can be expressed in terms of A:

$$A\xi = C(\xi - \ell) \tag{46}$$

$$\therefore C = A\xi/(\xi - \ell) \tag{47}$$

Substituting expression (47) back into (44), the Green's function takes the form

$$G(x,\xi) = \begin{cases} Ax & x < \xi \\ \dfrac{A\xi}{(\xi-\ell)}(x-\ell) & x > \xi \end{cases} \tag{48}$$

Using property (4), the fi[illegible] rivative of $G(x,\xi)$ must be discontinuous at $x=\xi$ [illegible] fically,

$$\left.\frac{dG_2(x)}{dx}\right|_{x\to\xi} - \left.\frac{dG_1(x)}{dx}\right|_{x\to\xi} = 1 \tag{49}$$

Doing the differentiation yields

$$\frac{A\xi}{(\xi-\ell)} - A = -1 \tag{50}$$

or

$$A = \frac{(\ell-\xi)}{\ell} \tag{51}$$

and equation (48) becomes

$$G(x,\xi) = \begin{cases} (\ell-\xi)\dfrac{x}{\ell} & x < \xi \\ (\ell-x)\dfrac{\xi}{\ell} & x > \xi \end{cases} \tag{52}$$

Equation (52) represents the final expression for $G(x,\xi)$ for the operator $L = \frac{d^2}{dx^2}$. Notice that this is exactly the form of the kernel for the integral expansion of this boundary value problem, given by equation (22).

The Green's Integral Equation

Many different boundary value problems, upon

integral conversion, have symmetric kernels equivalent to weighted Green's functions. Therefore, two procedures to generate the Green's function can be used:

(1) Through integral conversion or

(2) Finding $G(x,\xi)$ from the differential operator, L.

It should also be mentioned that not all integral conversions yield symmetric Green's functions. In particular, if the differential equation is of the form

$$\frac{d^2y}{dx^2} + A\frac{dy}{dx} + By = 0 \tag{53}$$

with homogeneous boundary conditions

$$y(0) = 0, \qquad y(\ell) = 0 \tag{54}$$

then the resulting kernel of the integral equation is both nonsymmetric and discontinuous at $x = \xi$, unless $A = 0$ (Appendix A).

Both methods (1) and (2) should be equivalent, however different expressions for $G(x,\xi)$ can occur. As an example consider the one-dimensional Helmholtz boundary value problem

$$\frac{d^2y}{dx^2} + \lambda^2 y = 1 \tag{55}$$

with boundary conditions

$$y(0) = 0, \qquad y(1) = 0 \tag{56}$$

Upon integral conversion, page 68, it was found that $y(x)$ was of the form

$$y(x) = \int_0^1 K(x,\xi)(\lambda^2 y(\xi) - 1)\, d\xi \tag{57}$$

where the kernel is defined by the expression

$$K(x,\xi) = \begin{cases} x(1-\xi) & x < \xi \\ \xi(1-x) & x > \xi \end{cases} \tag{58}$$

Expression (58) represents the equivalent weighted Green's function for the integral conversion method. Next, consider the problem in operator form, where L represents the one-dimensional Helmholtz operator

$$L = \frac{d^2}{dx^2} + \lambda^2 \tag{59}$$

The Green's function must obey the differential equation

$$\frac{d^2 G(x,\xi)}{dx^2} + \lambda^2 G(x,\xi) = -\delta(x-\xi) \tag{60}$$

From the method outlined using the differential operator, L, the Green's function was found to be (Appendix C):

$$G(x,\xi) = \begin{cases} \dfrac{\sin\lambda(\ell-\xi)}{\lambda\sin\lambda\ell}\sin\lambda x & x<\xi \\ \dfrac{\sin\lambda(1-x)}{\lambda\sin\lambda\ell}\sin\lambda\xi & x>\xi \end{cases} \tag{61}$$

and $y(x)$ is given by

$$y(x) = -\int_0^1 G(x,\xi)\, d\xi \tag{62}$$

where $G(x,\xi)$ is defined by equation (61) and $f(\xi) = -1$ from

(55). Clearly, $y(x)$ is represented equivalently by two completely independent forms of the Green's function; that is, equations (57) and (62), each with distinct, different kernels, must be equivalent expressions.

Equivalency of the Integral Equation and the Green's Integral

It will now be shown that equations (57) and (62) are identical expressions and that they both satisfy the one-dimensional Helmholtz differential equation. Equation (57) can be written in the form

$$y(x) = \int_0^x \xi(1-x)\{\lambda^2 y(\xi) - 1\}\, d\xi + \int_x^1 x(1-\xi)\{\lambda^2 y(\xi) - 1\}\, d\xi \tag{63}$$

where the kernel, defined by equation (58) has been substituted over the appropriate limits. According to Leibnitz's rule for differentiation under an integral, (Ref 1: 383), the first derivative of (63) becomes

$$y'(x) = -\int_0^x \xi(\lambda^2 y(\xi) - 1)\, d\xi + \int_x^1 (1-\xi)(\lambda^2 y(\xi) - 1)\, d\xi \tag{64}$$

The second derivative of $y(x)$ is found by differentiating (64) with respect to x, and is

$$y''(x) = -x(\lambda^2 y(x) - 1) - (1-x)(\lambda^2 y(x) - 1) = 1 - \lambda^2 y(x) \tag{65}$$

Substituting the equation for $y''(x)$, equation (65), back into the original differential equation, expression (55), it is found that

$$y''(x) + \lambda^2 y(x) = \left\{ 1 - \lambda^2 y(x) \right\} + \lambda^2 y(x) = 1 \tag{66}$$

Hence, the integral representation given by (57) satisfies differential equation (55) and therefore must be equivalent due to the uniqueness of solution guaranteed through the given boundary conditions.

Equation (62) can likewise be written in the form

$$y(x) = -\int_0^x \frac{\sin\lambda(\ell-x)\sin\lambda\xi}{\lambda\sin\lambda\ell}\, d\xi - \int_x^1 \frac{\sin\lambda(\ell-\xi)\sin\lambda x}{\lambda\sin\lambda\ell}\, d\xi \tag{67}$$

where again $G(x,\xi)$ has been substituted over its defined limits. Using Leibnitz's rule the first derivative of $y(x)$ becomes

$$y'(x) = \lambda\int_0^x \frac{\cos\lambda(\ell-x)\sin\lambda\xi}{\lambda\sin\lambda\ell}\, d\xi - \lambda\int_x^1 \frac{\cos\lambda x\sin\lambda(\ell-\xi)}{\lambda\sin\lambda\ell}\, d\xi \tag{68}$$

The second derivative, differentiating expression (68), becomes the quantity

$$y''(x) = \lambda^2\int_0^x \frac{\sin\lambda(\ell-x)\sin\lambda\xi}{\lambda\sin\lambda\ell}\, d\xi + \lambda^2\int_x^1 \frac{\sin\lambda x\sin\lambda(\ell-\xi)}{\lambda\sin\lambda\ell}\, d\xi$$

$$+ \frac{\lambda\cos\lambda(\ell-x)\sin\lambda x + \lambda\cos\lambda x\sin\lambda(\ell-x)}{\lambda\sin\lambda\ell} \tag{69}$$

Substituting the integral expression for $y''(x)$ and $y(x)$ back into the original differential equation, it is found that

$$y''(x) + \lambda^2 y(x) = \frac{\lambda\cos\lambda(\ell-x)\sin\lambda x + \lambda\cos\lambda x\sin\lambda(\ell-x)}{\lambda\sin\lambda\ell} \tag{70}$$

After simplifying, the right-hand side of equation (70) becomes

$$y''(x) + \lambda^2 y(x) = \frac{\lambda \sin \lambda \ell (\sin^2 \lambda x + \cos^2 \lambda x)}{\lambda \sin \lambda \ell} = 1 \tag{71}$$

Therefore, the Green's integral representation also satisfies differential equation (55) and both integral forms, equations (57) and (62) must be equivalent expressions.

Integral Representation

One last procedure will be introduced to demonstrate how equation (62) originates. Consider the two equations

$$\frac{d^2y}{dx^2} = -f(x), \quad y(0) = a, \; y(\ell) = b \tag{72}$$

and

$$\frac{d^2G(x,\xi)}{dx^2} = -\delta(x-\xi) \tag{73}$$

Equation (73) represents the Green's function solution for the differential operator $L = \frac{d^2}{dx^2}$. Multiply equation (72) by $G(x,\xi)$ and equation (73) by $y(x)$, subtract and integrate over the interval $(0,\ell)$ to obtain

$$\int_0^\ell \left\{ G(x,\xi)\frac{d^2y(x)}{dx^2} - y(x)\frac{d^2G(x,\xi)}{dx^2} \right\} dx =$$

$$-\int_0^\ell G(x,\xi) f(x)\,dx + \int_0^\ell y(x)\delta(x-\xi)\,dx \tag{74}$$

Rewriting the left-hand derivatives in equation (74) and using the integral properties of the Dirac delta function (Ref 5: 6), equation (74) becomes

$$\int_0^{\ell}\left\{G(x,\xi)\frac{d}{dx}\left(\frac{dy}{dx}\right)dx - y\frac{d}{dx}\left(\frac{dG(x,\xi)}{dx}\right)\right\}dx =$$

$$-\int_0^{\ell} G(x,\xi)\, f(x)\, dx + y(\xi) \tag{75}$$

Integrating the left side by parts, using the fact that

$$\int u\, dv = \int u\frac{dv}{dx}dx = uv - \int v\frac{du}{dx}dx \tag{76}$$

The left-hand side of equation (75) becomes

$$G(x,\xi)\frac{dy}{dx}\Big|_0^{\ell} - y\frac{d}{dx}G(x,\xi)\Big|_0^{\ell} - \int \cancel{\frac{dy}{dx}\frac{dG}{dx}}\,dx + \int \cancel{\frac{dG}{dx}\frac{dy}{dx}}\,dx \tag{77}$$

Evaluating at the limits, (77) becomes

$$G(\ell,\xi)\frac{dy(\ell)}{dx} - G(0,\xi)\frac{dy(0)}{dx} - y(\ell)\frac{dG}{dx}(x,\xi)\Big|_{x\to\ell} + y(0)\frac{dG}{dx}(x,\xi)\Big|_{x\to 0} \tag{78}$$

Because the Green's function is zero at end points the first two quantities on the left drop out. The only expressions left to evaluate are the derivatives of $\frac{dG(x,\xi)}{dx}$ on the appropriate intervals. Differentiating equation (52), which is the known $G(x,\xi)$ for the operator $\frac{d^2}{dx^2}$, gives

$$\frac{dG(x,\xi)}{dx} = \begin{cases} \frac{(\ell-\xi)}{\ell} & x < \xi \\ -\frac{\xi}{\ell} & x > \xi \end{cases} \tag{79}$$

Using $\frac{dG(x,\xi)}{dx}$ above, equation (78) becomes

$$\frac{y(\ell)\xi}{\ell} + \frac{y(0)(\ell-\xi)}{\ell} = -\int_0^{\ell} G(x,\xi)f(x)dx + y(\xi) \tag{80}$$

Solving for $y(\xi)$, and substituting the boundary conditions at $y(0)$ and $y(\ell)$, equation (80) becomes the expression

$$y(\xi) = \int_0^{\ell} G(x,\xi)f(x)dx + \frac{b\xi}{\ell} + \frac{a(\ell-\xi)}{\ell} \tag{81}$$

Interchanging the labels x and ξ from the Reciprocity principle (Ref 6: 328) and using the symmetry of $G(x,\xi)$, equation (81) is transformed into

$$y(x) = \int_0^{\ell} G(x,\xi)f(\xi)d\xi + \frac{bx}{\ell} + \frac{a(\ell-x)}{\ell} \tag{82}$$

This equation is the Green's integral solution of differential equation (72), with inhomogeneous Dirichlet boundary conditions. Note the similarity of this representation versus the integral equation expression given by equation (23).

Numerical Integration

An integral of the form $\int_a^b f(x)dx$ stands for the area represented by $f(x)$ over the interval (a,b). This area can be approximated by several methods; the trapezoid rule is based on linear interpolation, the integral is expressed as a sum of N trapezoidal areas; Simpson's rule for numerical integration is based upon

quadratic interpolation, parabolas or polynominals of degree 2 or less are used to approximate $f(x)$ between three successive points; the Newton-Cotes method is based upon polynominal interpolation of degree 3 or more. In this thesis the trapezoid rule is used to numerically integrate all one-dimensional cases.

Trapezoid Rule

The area of a typical trapezoid with base length h and sides $f(x_{i-1})$ and $f(x_i)$ is

$$Area = \frac{h}{2}\left[f(x_{i-1}) + f(x_i)\right] \tag{83}$$

The combined area of all trapezoids, over the interval $a = x_1$ to $b = x_N$ is

$$\text{Total area} = \frac{h}{2}[f(x_1)+f(x_2)] + \frac{h}{2}[f(x_2)+f(x_3)] + \cdots + \frac{h}{2}[f(x_{i-1})+f(x_i)] \tag{84}$$

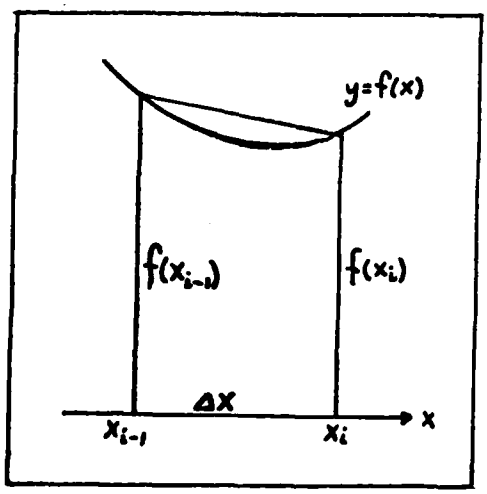

Fig. 2 Trapezoid Partition

Therefore, for the trapezoid rule equation (84) becomes

$$\int_a^b f(x)\,dx \cong \frac{h}{2}\left[f(x_1)+2f(x_2)+\cdots+2f(x_{N-1})+f(x_N)\right] \tag{85}$$

where $x_1, x_2, \ldots, x_N$ are equally spaced points dividing the interval from $a = x_1$ to $b = x_N$ into (N-1) equal parts, of length $h = (b-a)/(N-1)$. The trapezoid rule can be made as accurate as desired by choosing h very small, i.e., N very large. In addition, there are several advantages in using trapezoid interpolation versus the Simpson's rule.

Trapezoid vs. Simpson's Rule

It was shown earlier that all differential equations of the form

$$\frac{d^2y(x)}{dx^2} = -f(x) \tag{86}$$

with homogeneous end conditions have linear Green's kernels when expressed in integral form (Ref 1: 461-462). The linear kernel of equation (86) is shown in Fig. 1 and given by equation (22). Due to the linearity of $K(x,\xi)$ and the presence of a 'corner' at $x = \xi$, Simpson's rule for numerical integration will be less accurate than the trapezoid rule (Ref 7: 217, Problem #4-25). Trapezoids furnish better approximations to linear kernels than parabolas. Parabolas always exceed the actual area bounded by three consecutive points across

the discontinuity, at $x=\xi$, for a linear kernel. In addition, Simpson's rule can only be used if N, the number of points in the interval (a,b), is odd. By using Simpson's rule with N even the computed integral will exceed the true value because of the multiple contributions from trapezoids adjacent to the discontinuity. As an example to illustrate what happens by using Simpson's rule when N is even, consider the area bounded by the linear kernel given by equation (22) over the interval (0,1). The linear kernel is

$$K(x,\xi) = \begin{cases} x(1-\xi) & x < \xi \\ \xi(1-x) & x > \xi \end{cases} \tag{87}$$

Divide the interval (0,1) into three regions defined by the four equally spaced points

$$x_1 = 0, \qquad x_2 = 1/3, \qquad x_3 = 2/3, \qquad x_4 = 1$$

Fixing $\xi = 2/3$ and applying Simpson's rule to the area defined by $K(x,\xi)$, one extra contribution from the region defined over (x_2, x_3) is added into the total area.

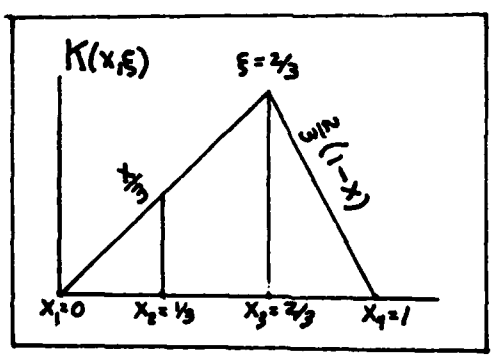

Fig. 3 The Linear Kernel, $K(x,\xi)$

The first contribution comes from applying quadratic interpolation over the first three points (x_1, x_2, x_3). Recall that in quadratic interpolation a polynominal of degree 2 or less is used to represent a function $f(x)$ over two successive intervals (x_1, x_2, x_3). Mathematically, if the value of $f(x)$ is known at three locations, a polynominal, $p(x)$, can be determined of the form

$$p(x) = Ax^2 + Bx + C \tag{88}$$

where A, B, and C are all constants to be determined from the three points

$$(x_1, f(x_1)), \quad (x_2, f(x_2)), \quad (x_3, f(x_3))$$

Once determined, $p(x)$ is then substituted for $f(x)$ over the interval (x_1, x_2, x_3) and integrated by expression (85). Over the points x_1, x_2, and x_3 given above, and using the value of $K(x,\xi)$ on the interval $x<\xi$, $p(x)$ can be found and is

$$p(x) = \frac{x}{3} \tag{89}$$

Therefore, Simpson's method applied to the first three points in Fig. 3 is the area represented under the line $K(x,\xi) = x/3$.

To calculate the remaining area under $K(x,\xi)$ for $x>\xi$, three additional points and the values of $f(x)$ must be known. Now however, only two points remain for the in-

terval $x > \xi$, x_3 and x_4. If x_2 is used again, in conjunction with x_3, and x_4, a parabola can be constructed to pass through all three points. The polynominal over the 'corner' of $K(x,\xi)$ defined on the interval (x_1, x_2, x_3) can be and is

$$p(x) = -\frac{9}{2}x^2 + \frac{11}{2}x - 1 \tag{90}$$

Hence, the area under the interval from x_2 to x_4 is added onto that already calculated from the first interval, adding in the area (x_2, x_3) twice. Not only is

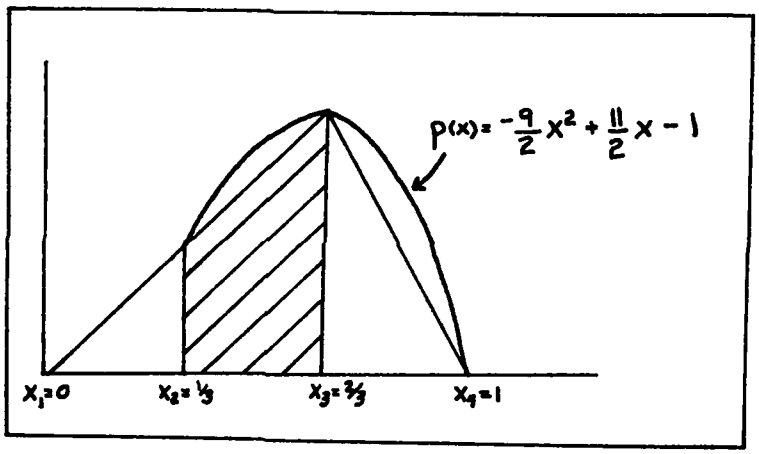

Fig. 4 Quadratic Interpolation Across the Discontinuity $\xi = 2/3$.

the area via Simpson's rule in error but note that by using parabolas a larger area is actually obtained since $p(x)$ encompasses the linear boundaries of $K(x,\xi)$. Even for N odd, parabolas still overestimate the desired area, and not until $K(x,\xi)$ is represented by a non-linear function does the Simpson's technique yield a more

accurate result compared to the trapezoid method.

Finite Difference Method

The method of finite differences is a process of numerical differentiation; the original differential equation is replaced by finite difference approximations. This technique converts the original differential equation into a system of linear algebraic expressions which can be solved simultaneously to give solutions at a finite number of points.

The differential operator by definition is expressed quantitatively as

$$\frac{dy}{dx} = \lim_{\Delta x \to 0} \frac{y(x+\Delta x) - y(x)}{\Delta x} \tag{91}$$

However, because the computer cannot take the limit one must approximate $\frac{dy}{dx}$ by using a small Δx, that is

$$\frac{dy}{dx} \cong \frac{y(x+\Delta x) - y(x)}{\Delta x} \tag{92}$$

This quanity is known as the first forward difference quotient. Expression (92) represents the change in some function by incrementing x a positive amount Δx.

The general procedure to obtain difference approximations for derivatives is to express several values of y at adjacent points in a Taylor series expansion, it is then possible to solve for the needed derivative through algebraic manipulation.

To derive the numerical analogy for the first and second derivatives, expand y in a Taylor series about the two points $x+h$ and $x-h$:

$$y(x+h) = y(x) + hy'(x) + \frac{h^2}{2}y''(x) + \frac{h^3}{6}y'''(x) + \cdots + O(h^4) \tag{93}$$

$$y(x-h) = y(x) - hy'(x) + \frac{h^2}{2}y''(x) - \frac{h^3}{6}y'''(x) + \cdots + O(h^4) \tag{94}$$

Adding equations (93) and (94), the sum becomes

$$y(x+h) + y(x-h) = 2y(x) + h^2y''(x) + \cdots + O(h^4) \tag{95}$$

where $O(h^4)$ refers to terms containing fourth and higher powers of h. By assuming the higher ordered terms are negligible compared to the lower powers of h, for small values of h, equation (95) can be solved for $y''(x)$, and is

$$y''(x) = \frac{y(x+h) - 2y(x) + y(x-h)}{h^2} + O(h^2) \tag{96}$$

As h becomes small the remainder terms can be neglected and (96) reduces to

$$y''(x) \cong \frac{y(x+h) - 2y(x) + y(x-h)}{h^2} \tag{97}$$

The above expression is known as the central finite difference (CFD) approximation to the second derivative of $y(x)$ and has an associated error of order h^2.

To approximate the first derivative, subtract equation (94) from (93) and obtain the quanity

$$y(x+h) - y(x-h) = 2h\,y'(x) + O(h^3) \tag{98}$$

or, solving for $y'(x)$

$$y'(x) = \frac{y(x+h) - y(x-h)}{2h} + O(h^2) \tag{99}$$

The central difference approximation for the first derivative is also of order h^2. For small values of h, $y'(x)$ becomes

$$y'(x) \cong \frac{y(x+h) - y(x-h)}{2h} \tag{100}$$

In addition to the central difference scheme it is also possible to approximate the derivative from two adjacent points, a distance h and $2h$ from x, the technique is known as the first forward difference (FFD) method. To find the first forward difference expression for the first derivative solve (93) for $y'(x)$

$$y'(x) = \frac{y(x+h) - y(x)}{h} + O(h) \tag{101}$$

Likewise, for the second derivative

$$y''(x) = \frac{y(x+2h) - 2y(x+h) + y(x)}{h^2} + O(h) \tag{102}$$

Note in the FFD methods the errors associated with equations (101) and (102) are of order h. For the CFD methods however, the errors are of order h^2. Therefore, it can be concluded that using points symmetrically located with respect to x give more accurate results, by a factor of h, than those based on the FFD techniques (Ref 8: 63).

Matrix Methods: The Integral Form of Solution

A definite integral of the form $y = \int_a^b f(x)dx$ can be written exactly as

$$y(x) = \lim_{N \to \infty} \sum_{K=1}^{N} f(x_K)(\Delta x_K) \tag{103}$$

where the interval (a,b) is divided into N subintervals of lengths $\Delta x_1, \ldots, \Delta x_N$, and x_K is a point of the Kth subinterval (Ref 1: 444). An approximation to (103) can be obtained by expressing $y(x)$ as a weighted sum of the ordinates $f(x_K)$ at N conveniently chosen points $x_1, x_2, \ldots, x_N$ on the interval (a,b), that is

$$y(x) \cong \sum_{K=1}^{N} D_K f(x_K) = D_1 f(x_1) + D_2 f(x_2) + \cdots + D_N f(x_N) \tag{104}$$

where D_K is a weighing coefficient associated with the point x_K. The coefficient D_K, when the points $x_1, x_2, \ldots, x_N$ are equally spaced, can be chosen in accordance with formulas for numerical integration, such as the trapezoid rule. Recall that use of the trapezoid rule for an integral gives

$$\int_a^b f(x)dx \cong \frac{h}{2}\left\{ f(x_1) + 2f(x_2) + \cdots + 2f(x_{N-1}) + f(x_N) \right\} \tag{105}$$

where $h = (b-a)/(N-1)$. Identifying the 'weighing' coefficients, D_K, with the trapezoid rule it is found that

$$\left\{ D_1, D_2, D_3, \cdots, D_{N-2}, D_{N-1}, D_N \right\} = \frac{h}{2}\left\{ 1, 2, 2, \cdots, 2, 2, 1 \right\} \tag{106}$$

In the same way integral equations such as

$$y(x) = F(x) + \int_a^b K(x,\xi)\, y(\xi)\, d\xi \tag{107}$$

can be approximated in the form

$$y(x) \cong F(x) + \sum_{k=1}^{N} D_k\, K(x,x_k)\, y(x_k) \tag{108}$$

where, again the points x_k are chosen at N locations in the interval (a,b). The D_k values correspond to weighing coefficients based upon the approximation method used, i.e., Simpson's or trapezoid rule. By requiring that both sides of equation (108) be equal at each of the N chosen points, N linear equations results

$$y(x_i) = F(x_i) + \sum_{k=1}^{N} D_k\, K(x_i,x_k)\, y(x_k) \qquad i = 1,2,\ldots,N \tag{109}$$

where the unknowns $y(x_1),\ldots,y(x_N)$ correspond to the values of the unknown function $y(x)$ at N locations. Introducing the abbreviations

$$y_i = y(x_i), \qquad F_i = F(x_i), \qquad K_{ij} = K(x_i,x_j) \tag{110}$$

where K_{ij} is the value of $K(x,\xi)$ when $x = x_i$ and $\xi = x_j$, expression (109) becomes

$$y_i = F_i + \sum_{k=1}^{N} K_{ij}\, D_k\, y_k \tag{111}$$

The kernel K_{ij} can be written in the form of a matrix

$$\bar{\bar{K}} = \begin{bmatrix} K(1,1) & K(1,2) & \cdots & K(1,N) \\ K(2,1) & & & \\ \vdots & & & \\ K(N,1) & & & K(N,N) \end{bmatrix} \tag{112}$$

Also, D_K can take the form of a diagonal matrix by defining $D_K = \left[D_K \delta_{iK} \right]$

$$\bar{\bar{D}} = \begin{bmatrix} D_1 & 0 & \cdots & \cdot \\ 0 & D_2 & & \\ \vdots & & \ddots & \\ & & & D_N \end{bmatrix} \tag{113}$$

Equation (111) can be expressed in matrix form as

$$\left[\bar{\bar{I}} - \bar{\bar{K}} \bar{\bar{D}} \right] \bar{y} = \bar{F} \tag{114}$$

where $\bar{\bar{I}}$ is the unit matrix of order N. The single bar denotes a column vector and the double bar a matrix quanity. Consequently the integral form of solution is expressed, for computer analysis, as a problem of matrix multiplication.

Matrix Methods: The Method of Finite Differences

Just as was the case with the integral conversion, it is also possible to transform the method of finite differences into a problem of matrix multiplication.

Consider the general second order differential equation

$$\frac{d^2y}{dx^2} + f(x)\frac{dy}{dx} + g(x)y = r(x) \tag{115}$$

with boundary conditions

$$y(x_1) = A, \qquad y(x_N) = B \tag{116}$$

Using central finite differences, the first and second derivatives of $y(x)$ can be approximated by equations (92) and (97). Substituting these quantities and combining terms, equation (115) becomes

$$y(x-h)\left\{1 - \frac{f(x)h}{2}\right\} + y(x)\left\{h^2 g(x) - 2\right\}$$

$$+ y(x+h)\left\{1 + \frac{f(x)h}{2}\right\} = r(x)h^2 \tag{117}$$

Once again introduce the notation

$$y_i = y(x_i), \quad F_i = 1 - \frac{f(x_i)h}{2}, \quad G_i = h^2 g(x_i) - 2,$$

$$E_i = 1 + \frac{f(x_i)h}{2}, \quad R_i = r(x_i)h^2 \tag{118}$$

Equation (117) becomes equivalent to the system of linear equations

$$y_{i-1}F_i + y_i G_i + y_{i+1}E_i = R_i \qquad (i = 2, 3, \cdots, N-1) \tag{119}$$

If the end conditions, $y_1 = A$ and $y_N = B$, are substituted (119) can be expressed as the system of equations defined from $i = 2, 3, \cdots, N-1$:

$$
\left.
\begin{array}{lrcl}
i=2 & AF_2 + y_2G_2 + y_3E_2 & = & R_2 \\
i=3 & y_2F_3 + y_3G_3 + y_4E_3 & = & R_3 \\
i=4 & y_3F_4 + y_4G_4 + y_5E_4 & = & R_4 \\
\vdots & & & \\
i=N-1 & y_{N-2}F_{N-1} + y_{N-1}G_{N-1} + BE_{N-1} & = & R_{N-1}
\end{array}
\right\} \quad (120)
$$

and rewritten in matrix form as

$$
\begin{bmatrix}
G_2 & E_2 & 0 & \cdot & \cdot \\
F_3 & G_3 & E_3 & 0 & \\
0 & F_4 & G_4 & E_4 & \\
\cdot & & & & \\
\cdot & & & F_{N-1} & G_{N-1}
\end{bmatrix}
\begin{bmatrix}
y_2 \\ y_3 \\ y_4 \\ \vdots \\ y_{N-1}
\end{bmatrix}
=
\begin{bmatrix}
R_2 - AF_2 \\ R_3 \\ R_4 \\ \vdots \\ R_{N-1} - BE_{N-1}
\end{bmatrix}
\quad (121)
$$

The left-hand matrix in equation (121) is known as a tridiagonal matrix. The elements on the principle diagonal, super-diagonal, and sub-diagonal, are non-zero, with zero elements everywhere else (Ref 9: 104). Expression (121) can be written in the more concise matrix form

$$
\bar{\bar{B}}\,\bar{y} = \bar{R} \quad (122)
$$

where $\bar{\bar{B}}$ corresponds to the tridiagonal coefficient

matrix, and $\bar{y}$ and $\bar{R}$ are the perspective matrix vectors. Again, the differential form of solution is expressed, for computer analysis, as a problem of matrix multiplication.

Simultaneous Solution of Linear Equations

The solution for a system of equations, $\bar{\bar{A}}\bar{x} = \bar{b}$ is most efficiently solved by eliminating the unknowns, and the most commonly employed method is the Gauss elimination process. Consider as an example the following set of four equations:

$$\begin{bmatrix} C_{11} & C_{12} & C_{13} & C_{14} \\ C_{21} & C_{22} & C_{23} & C_{24} \\ C_{31} & C_{32} & C_{33} & C_{34} \\ C_{41} & C_{42} & C_{43} & C_{44} \end{bmatrix} \begin{bmatrix} X_1 \\ X_2 \\ X_3 \\ X_4 \end{bmatrix} = \begin{bmatrix} r_1 \\ r_2 \\ r_3 \\ r_4 \end{bmatrix} \tag{123}$$

The solution vector, $\bar{X}$, is the desired quanity and will be obtained through algebraic manipulation of the coefficient matrix in (123). During the process of this matrix manipulation it should be remembered that the solution of $\bar{X}$ remains unchanged if any of the following operations are preformed:

(1) Multiplication or division of any equation by a constant.
(2) Replacement of any equation by the sum or difference of that equation and any other equation.

Gauss elimination is simply a sequential application of the row operations (1) and (2) above. In

the algorithm, the top equation is first divided by C_{11}

$$\begin{bmatrix} 1 & C'_{12} & C'_{13} & C'_{14} \\ C_{21} & C_{22} & C_{23} & C_{24} \\ C_{31} & C_{32} & C_{33} & C_{34} \\ C_{41} & C_{42} & C_{43} & C_{44} \end{bmatrix} \begin{bmatrix} X_1 \\ X_2 \\ X_3 \\ X_4 \end{bmatrix} = \begin{bmatrix} r'_1 \\ r_2 \\ r_3 \\ r_4 \end{bmatrix} \tag{124}$$

where the primes denote elements whose values have been changed. The first equation is now multiplied by C_{21} and subtracted from the second to eliminate element C_{21}. Likewise the first equation can also be multiplied by C_{31} and subtracted from the third equation, then multiplied by C_{41} and subtracted from the fourth. In this manner the entire first column below C_{11} has been cleared to zero and the set appears as

$$\begin{bmatrix} 1 & C'_{12} & C'_{13} & C'_{14} \\ 0 & C'_{22} & C'_{23} & C'_{24} \\ 0 & C'_{32} & C'_{33} & C'_{34} \\ 0 & C'_{42} & C'_{43} & C'_{44} \end{bmatrix} \begin{bmatrix} X_1 \\ X_2 \\ X_3 \\ X_4 \end{bmatrix} = \begin{bmatrix} r'_1 \\ r'_2 \\ r'_3 \\ r'_4 \end{bmatrix} \tag{125}$$

During the column manipulation, the first row is termed the pivot row and C_{11} the pivot element. The second row now becomes the pivot row and C'_{22} the pivot element. The second equation is divided by C'_{22} to make the main diagonal element 1. Multiplication of the second equation by C'_{32} and subtraction from the third, and then multiplication by C'_{42} and subtraction

from the fourth, clears the second column below the main diagonal to zero. Similar operations with the third and fourth rows as pivot rows finally yield

$$\begin{bmatrix} 1 & c_{12}^* & c_{13}^* & c_{14}^* \\ 0 & 1 & c_{23}^* & c_{24}^* \\ 0 & 0 & 1 & c_{34}^* \\ 0 & 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{bmatrix} = \begin{bmatrix} r_1^* \\ r_2^* \\ r_3^* \\ r_4^* \end{bmatrix} \tag{126}$$

where the stars indicate elements which have been modified several times from their original values. Gauss elimination is sometimes called triangularization because the coefficient matrix is upper triangular, i.e., elements above the main diagonal are non-zero while those below equal zero. The bottom equation in (126) now directly gives the value of x_4 as

$$x_4 = r_4^* \tag{127}$$

The third equation is

$$x_3 + c_{34}^* x_4 = r_3^* \tag{128}$$

Because x_4 is known, x_3 can be solved to yield

$$x_3 = r_3^* - c_{34}^* x_4 = r_3^* - c_{34}^* r_4^* \tag{129}$$

Repeated back substitutions will evaluate one new unknown from each new equation. The unknown vector $\bar{x}$ will have been completely determined when the top equa-

tion is solved for X_1.

It should be mentioned that one computational difficulty can arise with the Gauss elimination technique. The pivot element in each row is the element on the main diagonal. By the time any given row becomes the pivot row, the main diagonal element in that row, i.e., the pivot element, will have been modified from its original value several times over. Under certain circumstances, the diagonal element can become very small in magnitude compared to the rest of the elements in that row, as well as inaccurate. This can result in an erroneous solution vector. The problem can be effectively treated by interchanging the columns of the matrix to shift the largest elements (in magnitude) in the pivot row into the diagonal position. The largest element then becomes the pivot element. With each new pivot row the operation is repeated. This scheme is known as partial pivoting and minimizes the roundoff errors.

In addition, it is important to note the two different types of coefficient matrices which can be encountered. For the integral solution the system of N algebraic equations will have a 'dense' NxN coefficient matrix, few zero off diagonal elements.

The solution of algebraic equations for the finite difference technique yields a banded coefficient matrix and is 'sparse', many zero off diagonal ele-

ments. These sets commonly arise in the numerical solution of partial differential equations and in the use of finite differences. Solutions of banded systems are considerably easier than those for full, dense coefficient matrices.

As an example, consider this set having a tri-diagonal coefficient matrix:

$$\begin{bmatrix} b_1 & c_1 & 0 & \cdot & \cdot & \cdot \\ a_2 & b_2 & c_2 & 0 & \cdot & \cdot \\ 0 & a_3 & b_3 & c_3 & 0 & \\ \cdot & & & \cdot & & \\ \cdot & & & & \cdot & \\ \cdot & & & a_{N-1} & b_{N-1} & c_{N-1} \\ & & & & a_N & b_N \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ \cdot \\ \cdot \\ x_{N-1} \\ x_N \end{bmatrix} = \begin{bmatrix} r_1 \\ r_2 \\ r_3 \\ \cdot \\ \cdot \\ r_{N-1} \\ r_N \end{bmatrix} \tag{130}$$

where the main diagonal elements are denoted as b, and the diagonal elements below and above the main diagonal are a and c respectively.

Applying Gauss elimination to (130) only one element (one of the a's) will be eliminated in each column because all remaining entries below the main diagonal are zero. Also, no entries outside the tri-diagonal band are changed from zero in the course of the elimination process. After the bottom row has been reached (130) becomes

$$\begin{bmatrix} 1 & c_1' & 0 & \cdots & & \\ 0 & 1 & c_2' & 0 & & \\ \cdot & 0 & 1 & c_3' & & \\ \cdot & & & \ddots & & \\ \cdot & & & & \ddots & \\ & & & & 1 & c_{N-1} \\ & & & & & 1 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ \vdots \\ x_{N-1} \\ x_N \end{bmatrix} = \begin{bmatrix} r_1' \\ r_2' \\ r_3' \\ \vdots \\ r_{N-1}' \\ r_N' \end{bmatrix} \tag{131}$$

From the bottom row, $x_N = r_N'$ and back substitutions yield the remaining unknowns.

What is important to note about the solution of this tridiagonal set is that the number of basic arithmetic operations is of order N, in contrast to the N^3 operations required for a full matrix. Not only does this small set of operations result in short computation times, but it also tends to minimize round-off errors. It is also much easier to store the entire coefficient matrix since only the three diagonal vectors $\mathbf{a}$, $\mathbf{b}$, and $\mathbf{c}$ are required (Ref 10: 90-98).

III. One-Dimensional Problems

Computer Programs

The computer programs written for all one-dimensional cases were very similar; the programs used common expressions, symbols, and followed parallel sequences so that minimum alterations were necessary to adapt each routine to new cases. The flow diagrams for both numerical integration and differentiation appears in Figure 5.

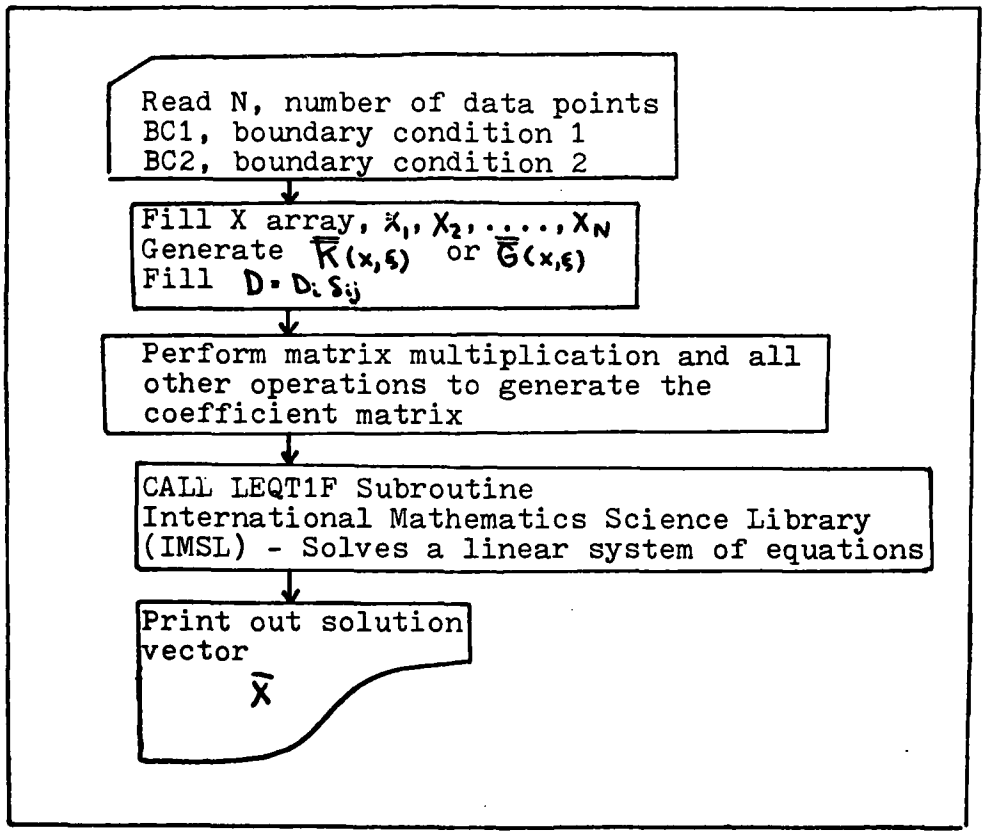

Fig. 5 Flow Diagram for Computer Programs Using Numerical Integration/Differentiation

Because the system of matrix equations are very similar, i.e., expressions (114) and (122), the only modification between the two programs were in the coefficient matrices. For numerical integration, the coefficient array was computed from matrix multiplication with the Green's kernel, $K(x,\xi)$, and the weighing coefficient, D_K. In the finite difference method however, the coefficient array was filled directly because of the simple band structure simply by noting the sequential arrangement of internal terms.

LEQT1F - IMSL Subroutine

The International Mathematics Science Library (IMSL) routine LEQT1F was used to solve all linear algebraic equations generated in the matrix formulations. LEQT1F solves the set of linear equations $\bar{\bar{A}}\bar{X} = \bar{B}$ for $\bar{X}$, given the NxN matrix $\bar{\bar{A}}$ and Nx1 matrix $\bar{B}$. The solution $\bar{X}$ will be the exact solution without any roundoff error. If such a solution cannot be obtained a warning is given. LEQT1F performs Gauss elimination and uses partial pivoting of the array elements.

Case I

The first problem addressed in this thesis, expressed mathematically is

$$\frac{d^2y(x)}{dx^2} = -y(x) \tag{132}$$

where $y(x)$ is the inhomogeneous term, with boundary conditions

$$y(0) = 0, \qquad y(1) = 1 \tag{133}$$

Analytical Solution

Equation (132) is equivalent to

$$\frac{d^2y(x)}{dx^2} + y(x) = 0 \tag{134}$$

and can be solved in a straightforward manner by assuming $y(x)$ to be a linear combination of the exponential function, that is

$$y(x) = e^{Dx} \tag{135}$$

Substituting (135) into (134) and dividing by e^{Dx} yields

$$D^2 + 1 = 0, \qquad \therefore\ D = \pm i \tag{136}$$

Using the two roots for D, the solution to (134) becomes

$$y(x) = Ae^{+ix} + Be^{-ix} = A'\cos x + B'\sin x \tag{137}$$

By applying the boundary conditions, $y(0)=0$ and $y(1)=1$, the constants A' and B' are evaluated. The complete

solution is found to be

$$y(x) = \frac{\sin x}{\sin 1} \tag{138}$$

and is graphed in Figure 6.

Integral Solution

To convert differential equation (132) into integral form, first integrate both sides of (132) with respect to x over the interval $(0,x)$

$$\int_0^x \frac{d}{dx}\left(\frac{dy}{dx}\right)dx = -\int_0^x y(x)\,dx \tag{139}$$

or

$$\frac{dy(x)}{dx} = C - \int_0^x y(x)\,dx \tag{140}$$

where the constant C is from the lower limit, $\frac{dy(0)}{dx}$. A second integration over the same interval and using equation (6) for the right-hand side, equation (140) becomes

$$y(x) = Cx - \int_0^x (x-\xi)\,y(\xi)\,d\xi \tag{141}$$

The constant C can be evaluated from the boundary condition $y(1)=1$ and equation (141) takes the form

$$y(x) = x + \int_0^1 K(x,\xi)\,y(\xi)\,d\xi \tag{142}$$

where the kernel is defined as the function

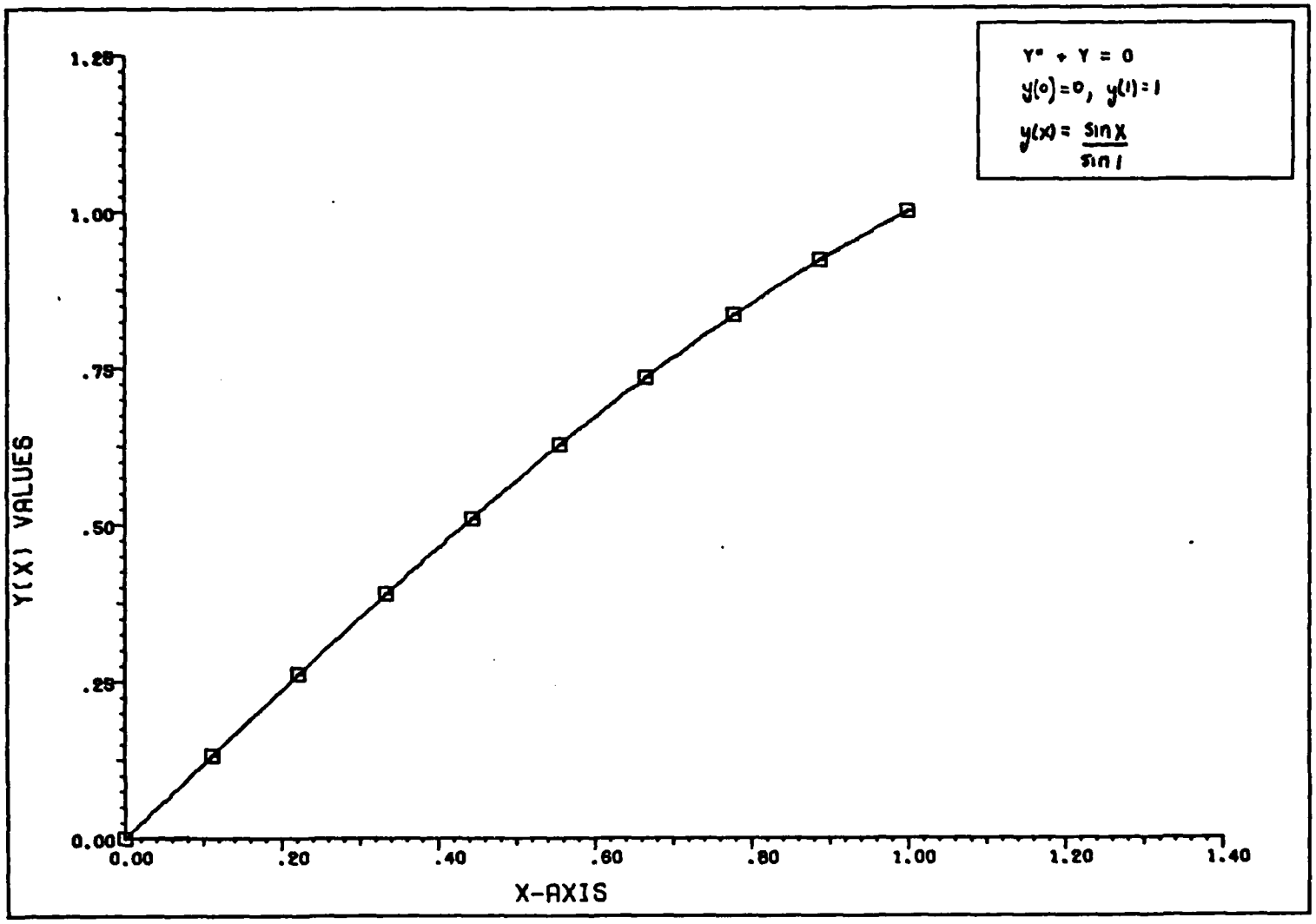

Fig. 6 Analytic Solution, Case I

$$K(x,\xi) = \begin{cases} x(1-\xi) & x < \xi \\ \xi(1-x) & x > \xi \end{cases} \tag{143}$$

Rearranging terms, (132) becomes equivalent to the expression

$$y(x) - \int_0^1 K(x,\xi)y(\xi)d\xi = x \tag{144}$$

Now, use the approximation for trapezoid integration for the integral and (144) becomes

$$y(x) - \sum_{k=1}^{N} D_k K(x,x_k)\, y(x_k) = x \tag{145}$$

Expressing D_k and $K(x,x_k)$ as matrices, equation (145) is transformed into the system of equations

$$\bar{y} - \bar{\bar{K}}\bar{\bar{D}}\bar{y} = \bar{x} \tag{146}$$

or

$$(\bar{\bar{I}} - \bar{\bar{K}}\bar{\bar{D}})\bar{y} = \bar{x} \tag{147}$$

For the case where the interval (0,1) is divided into four equal partitions, N=5, at

$$x_1 = 0, \quad x_2 = 1/4, \quad x_3 = 1/2, \quad x_4 = 3/4, \quad x_5 = 1$$

the matrix equation (147) takes the form

$$\left\{ \begin{bmatrix} 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 \end{bmatrix} - \begin{bmatrix} 0 & 0 & 0 & 0 & 0 \\ 0 & K & K & K & 0 \\ 0 & K & K & K & 0 \\ 0 & K & K & K & 0 \\ 0 & 0 & 0 & 0 & 0 \end{bmatrix} \begin{bmatrix} \frac{h}{2} & 0 & 0 & 0 & 0 \\ 0 & h & 0 & 0 & 0 \\ 0 & 0 & h & 0 & 0 \\ 0 & 0 & 0 & h & 0 \\ 0 & 0 & 0 & 0 & \frac{h}{2} \end{bmatrix} \right\} \begin{bmatrix} y_1 \\ y_2 \\ y_3 \\ y_4 \\ y_5 \end{bmatrix}$$

$$= \begin{bmatrix} 0 \\ 1/4 \\ 1/2 \\ 3/4 \\ 1 \end{bmatrix} \tag{148}$$

and the five linear equations from (148) are

$$\left. \begin{aligned} y_1 &= 0 \\ \tfrac{61}{64} y_2 - \tfrac{1}{32} y_3 - \tfrac{1}{64} y_4 &= 1/4 \\ -\tfrac{1}{32} y_2 + \tfrac{15}{16} y_3 - \tfrac{1}{32} y_4 &= 1/2 \\ -\tfrac{1}{64} y_2 - \tfrac{1}{32} y_3 + \tfrac{61}{64} y_4 &= 3/4 \\ y_5 &= 1 \end{aligned} \right\} \tag{149}$$

Solution of this set, rounded to six decimals, is

$$y_1 = 0, \quad y_2 = .294274, \quad y_3 = .570156, \quad y_4 = .810403, \quad y_5 = 1$$

The true values obtained from the analytical solution, equation (138), are

$$y_1 = 0, \quad y_2 = .294014, \quad y_3 = .569747, \quad y_4 = .810056, \quad y_5 = 1$$

<u>Finite Differences</u>

In a similar manner as was done to the integral equation, the method of finite differences is now applied to the original differential equation. By substituting the second derivative CFD quotient, equation (97), back into the original differential equation

for $y''(x)$, and collecting terms, equation (132) takes the form

$$y_{i-1} + (h^2-2)y_i + y_{i+1} = 0 \qquad i = 2,3,\ldots,N-1 \qquad (150)$$

where N is the number of points over the interval (0,1) and h, the interval spacing. A set of linear equations can be generated from (150) by letting i run through its sequence up to the value N-1. For N=5 and using the same five points as before, the central finite difference method will give the following set of linear equations:

$$\begin{aligned} y_1 - \tfrac{31}{16}y_2 + y_3 \qquad\qquad &= 0 \\ y_2 - \tfrac{31}{16}y_3 + y_4 \qquad &= 0 \\ y_3 - \tfrac{31}{16}y_4 + y_5 &= 0 \end{aligned} \qquad (151)$$

or in matrix form

$$\begin{bmatrix} 1 & -\frac{31}{16} & 1 & 0 & 0 \\ 0 & 1 & -\frac{31}{16} & 1 & 0 \\ 0 & 0 & 1 & -\frac{31}{16} & 1 \end{bmatrix} \begin{bmatrix} y_1 \\ y_2 \\ y_3 \\ y_4 \\ y_5 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix} \qquad (152)$$

Using the initial boundary conditions, $y_1 = 0$ and $y_5 = 1$, the following values, correct to six decimal places, are obtained for $y(x)$:

$y_1 = 0$, $y_2 = .294274$, $y_3 = .570156$, $y_4 = .810403$, $y_5 = 1$

Note that the same values were obtained using the trapezoid rule for numerical integration.

First Forward Difference

Besides the method of central finite differences, the first forward difference expression, equation (102), was substituted into (132) for a comparison of the two difference methods. Equation (132) now becomes

$$y_i(1+h) - 2y_{i+1} + y_{i+2} = 0 \qquad i = 1, 2, \ldots, N-2 \tag{153}$$

Again, for the same five points, (153) generates the linear equations

$$\begin{aligned} \tfrac{17}{16} y_1 - 2y_2 + y_3 \qquad\qquad &= 0 \\ \tfrac{17}{16} y_2 - 2y_3 + y_4 \qquad &= 0 \\ \tfrac{17}{16} y_3 - 2y_4 + y_5 &= 0 \end{aligned} \tag{154}$$

or the equivalent banded matrix

$$\begin{bmatrix} \frac{17}{16} & -2 & 1 & 0 & 0 \\ 0 & \frac{17}{16} & -2 & 1 & 0 \\ 0 & 0 & \frac{17}{16} & -2 & 1 \end{bmatrix} \begin{bmatrix} y_1 \\ y_2 \\ y_3 \\ y_4 \\ y_5 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix} \tag{155}$$

This set of equations, correct to six decimal places, has the solution

$y_1 = 0$, $y_2 = .266667$, $y_3 = .533333$, $y_4 = .783333$, $y_5 = 1$

For a comparison of the relative errors associated with

each of the two difference methods see Figure 7. The relative error data is displayed in Table I.

Error Analysis

It will be assumed that the major sources of error in all computed solutions is strictly associated

Table I. Relative Error (%) - Computer Solution for $y''+y=0$, $x=.5$

Number of Iterations per Interval	Integral Method	CFD Method	FFD Method
2	-.291500	-.291500	12.241744
4	-.071775	-.071775	6.391493
6	-.031741	-.031741	4.263721
8	-.017823	-.017823	3.109384
50	-.000455	-.000455	—

with the particular method being employed. All other error sources, such as truncation and internal round-off, due to the arithmetic process, are insignificant when compared to the errors created by a specific routine. By neglecting these other errors it will be possible to predict how large an error should occur and compare this to that actually observed.

Integral Equations

The error bound using the trapezoid rule (Ref 12: 405-408) is given by the expression

$$\frac{(b-a)Mh^2}{12} \geq \left| \int_a^b f(\xi)\,d\xi - T \right| \qquad (156)$$

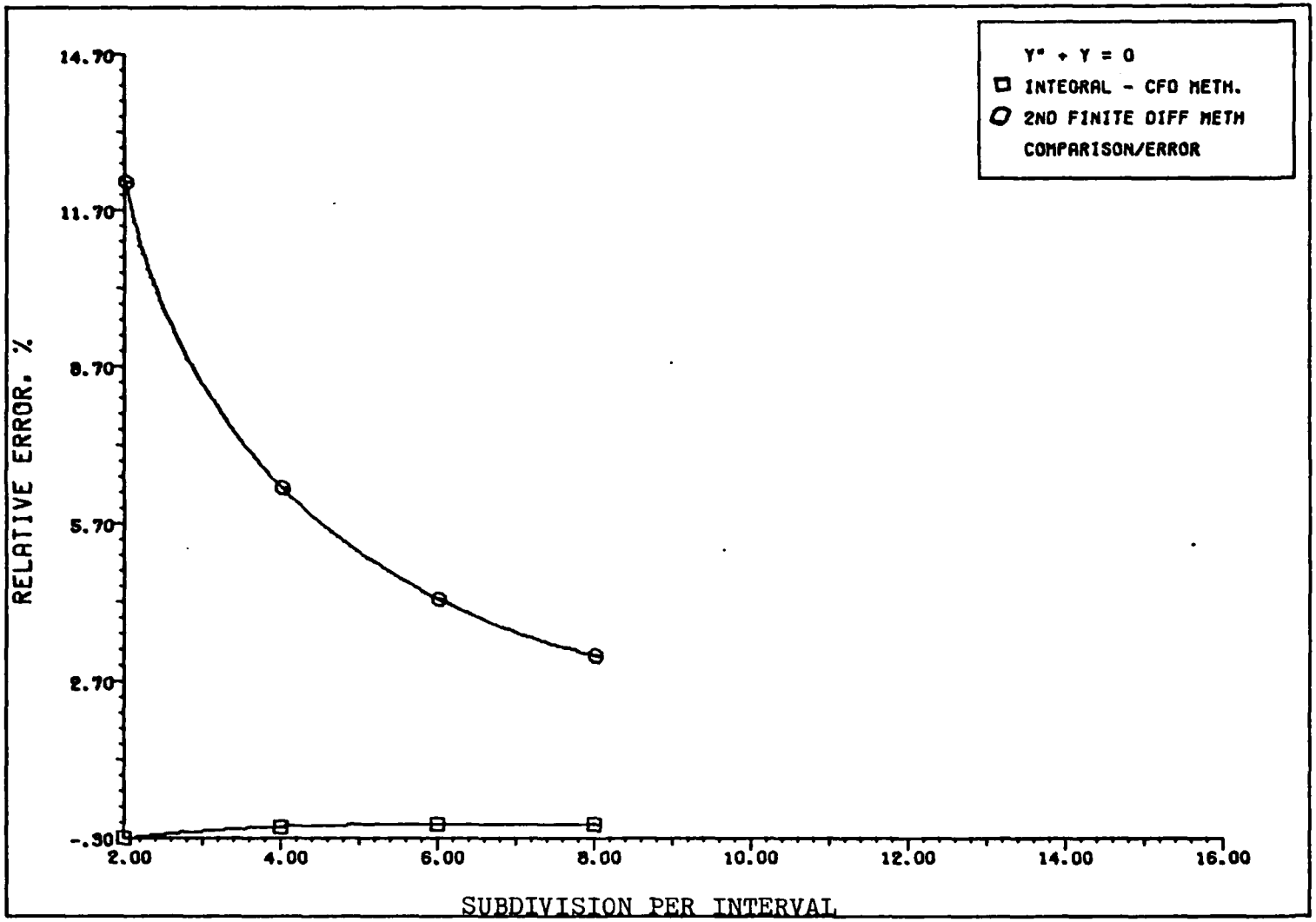

Fig. 7 Comparison of Relative Errors

where $\int_a^b f(\xi)\,d\xi$ is the required integral

T - number calculated via trapezoid rule

$(b-a)$ - the boundary interval

h - increment size

M - upper bound satisfying the condition

$$M \geq |f''(\xi)| \tag{157}$$

To predict how accurate the trapezoid rule is, the upper bound M must first be found. Again, it will be assumed that the only error in the integral solution of equation (144) is that due to numerically approximating the integral:

$$\int_0^1 K(x,\xi)\,y(\xi)\,d\xi \tag{158}$$

which, inserting the appropriate limits, becomes equivalent to two integrals:

$$\int_0^x \xi(1-x)\,y(\xi)\,d\xi + \int_x^1 x(1-\xi)\,y(\xi)\,d\xi \tag{159}$$

The error will be computed at the point $x = \frac{1}{2}$ since a number of values from Table I exist for comparison. Substituting $x = \frac{1}{2}$ expression (159) becomes

$$\int_0^{1/2} \frac{\xi\,y(\xi)}{2}\,d\xi + \int_{1/2}^1 \tfrac{1}{2}(1-\xi)\,y(\xi)\,d\xi \tag{160}$$

The function $f(\xi)$, from expression (156), can be taken as the sum of both integrands above; that is

$$f(\xi) = f_1(\xi) + f_2(\xi) \tag{161}$$

where

$$f_1(\xi) = \frac{\xi\, y(\xi)}{2} \quad \text{and} \quad f_2(\xi) = \frac{(1-\xi)}{2}\, y(\xi) \tag{162}$$

Taking the second derivative of $f(\xi)$ and substituting this quanity back into (157) will yield the bound M. It is found that

$$f''(\xi) = \frac{y(\xi)}{2} \tag{163}$$

The bound M is therefore

$$M \geq |f''(\xi)| = \frac{y(\xi)}{2} \tag{164}$$

The function $y(\xi)$ has its maximum value at $\xi = 1$ and $y(\xi)$ has the value of 1, from Figure 6. Therefore, M will be the upper bound

$$M = 1/2 \tag{165}$$

The total error at the point $x = 1/2$, using trapezoid rule, becomes

$$\text{Total error} = \frac{(b-a)Mh^2}{12} = \frac{h^2}{24} \tag{166}$$

As h is decreased the associated error should also decrease by a factor of h^2. This trend is indeed observed in the integral solution values shown in Table II.

Simpson's Comparison

In addition to use of the trapezoid rule, Simpson's

Table II. Error Trends Using Trapezoid Rule, x=.5

Increment Size h	y(x) Exact	y(x) Calculated	Actual Error	Calculated Error
1/2	.569747	.571429	-.001682	.0104167
1/4	.569747	.570156	-.000409	.0026042
1/6	.569747	.569928	-.000181	.0011574
1/8	.569747	.569849	-.000102	.0006510
1/50	.569747	.569750	-.000003	.0000167

rule for numerical integration was also used on (134). An interesting though not unpredictable trend was noticed in the data, Figure 8.

For $h = 1/50$, the computed array elements corresponding to the even intervals, i.e., odd array numbers were Simpson's method can be used, showed much smaller error values as compared to the even array elements. Also, as the array elements increased the relative error values decreased over both odd and even elements. The relative error is high at the even array elements due to the additional sum from an extra partition near the 'corner' in the quadratic interpolation scheme. The effect is to change the true area by an amount of the previous partitions area. The relative error values decrease because the partition areas decrease after the middle value, $\xi = 1/2$. For the lower points on Figure 8, where Simpson's rule is legal, the parabolas tend to approximate the kernel closer and have less overlap across the 'corner' sections of $K(x,\xi)$. The

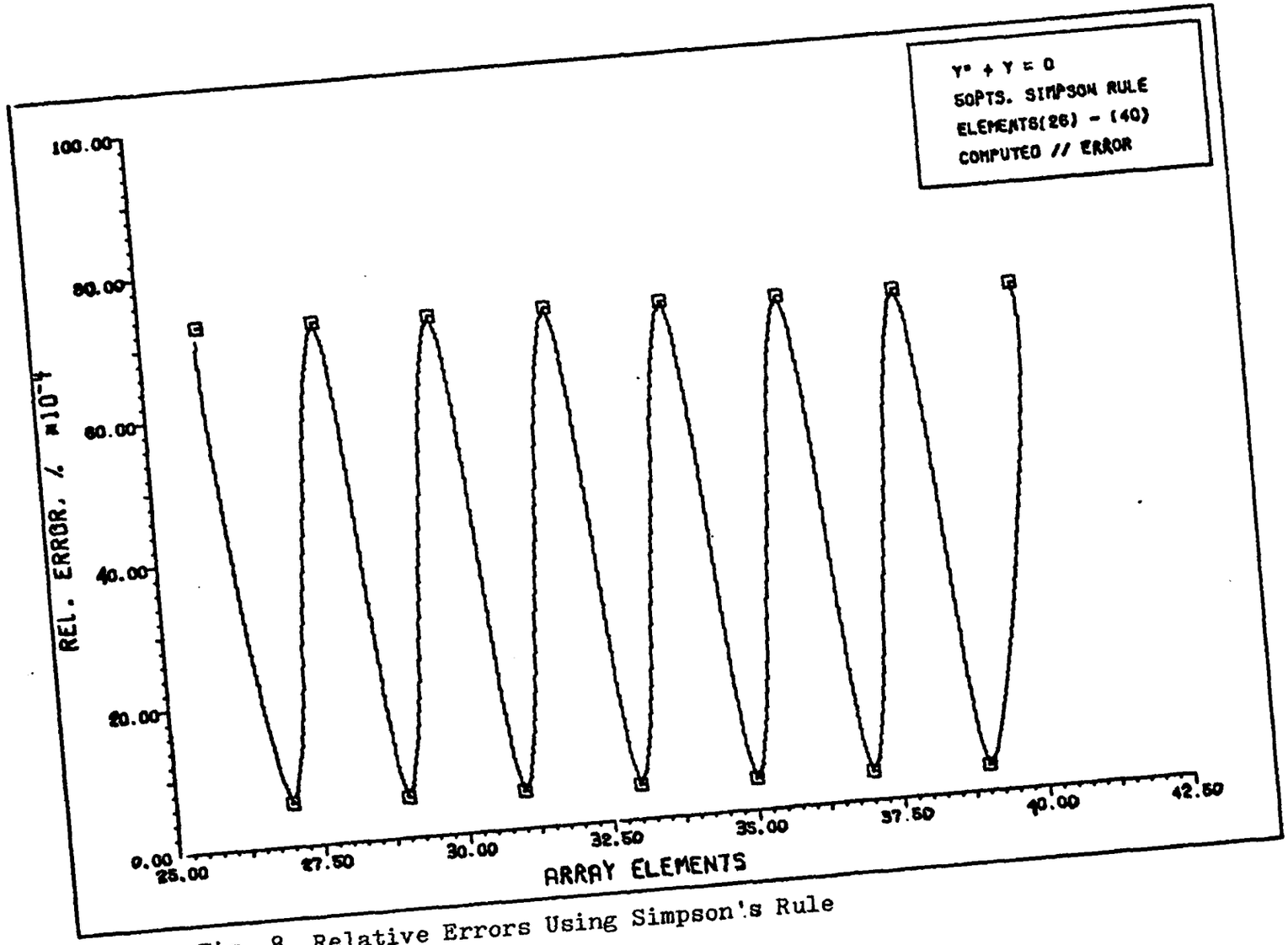

Fig. 8 Relative Errors Using Simpson's Rule

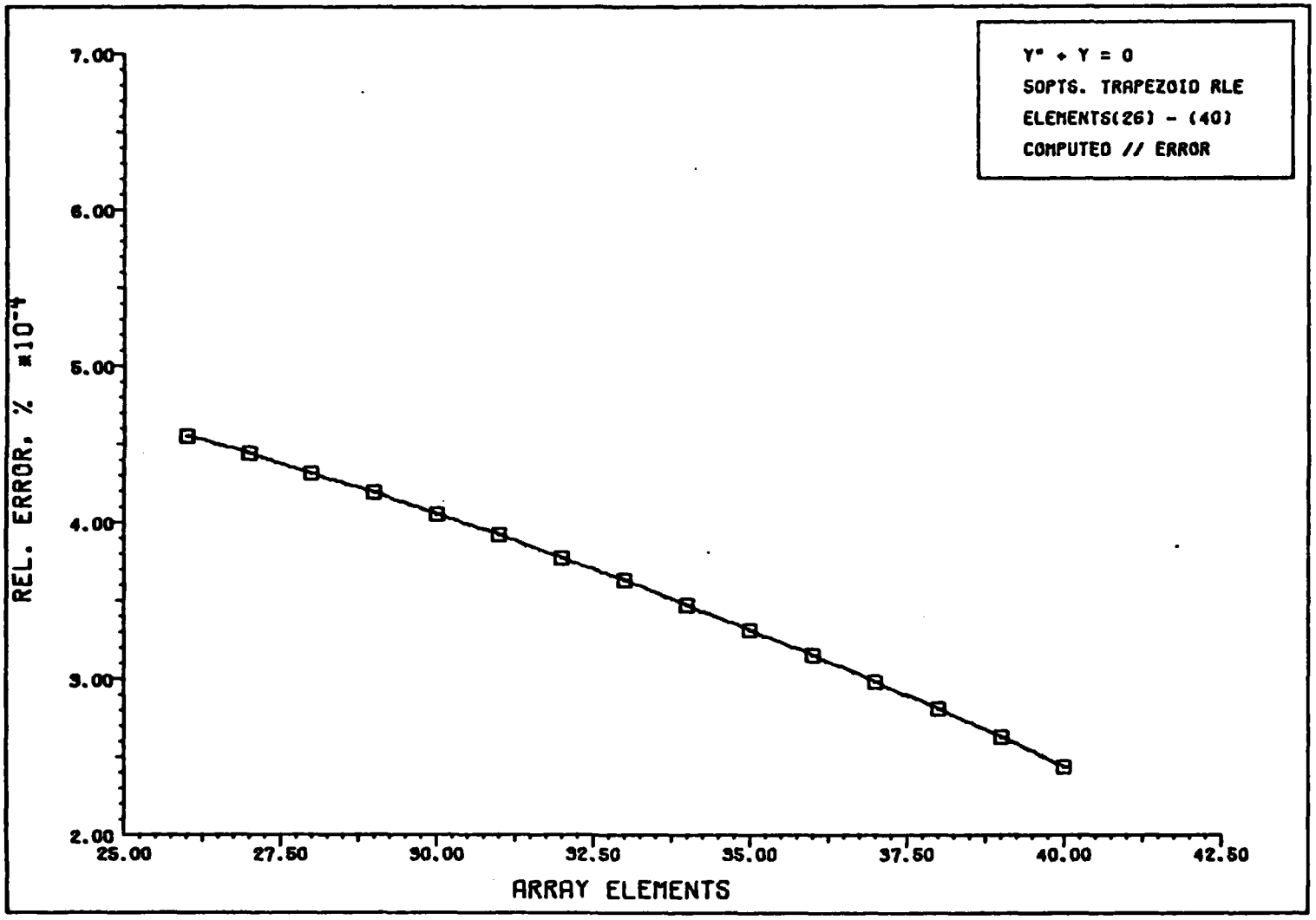

Fig. 9 Relative Errors Using Trapezoid Rule

relative errors for the same array elements using the trapezoid rule is shown in Figure 9.

Finite Differences

The major errors associated with the finite difference methods are from truncations in the Taylor series expansions used for $y(x)$. These errors can be reduced by taking more terms in the series expansion, however doing so does not necessarily guarantee numerical stability. Because of these facts it is extremely difficult to predict the relative size of error which should result from using the finite difference method. The error is carried in all linear equations generated by the recurrsion expression; when the number of equations becomes large, the resulting error combinations become exceedingly complicated. It is possible however to note the error trends in both the CFD and FFD methods.

Recall that the CFD method was of order $O(h^2)$, terms of order h^2 and higher were neglected in the central difference quotient, the second derivative became

$$y''(x) = \frac{y(x-h) - 2y(x) + y(x+h)}{h^2} + O(h^2) \cong \frac{y(x-h) - 2y(x) + y(x+h)}{h^2} \qquad (167)$$

It is reasonable to assume that errors associated with this method are as a direct result from neglecting the truncated terms of order h^2 and higher; therefore, the trend of error should be of order h^2. The

error trends using the central and first forward difference quotient are compared in Table III.

Table III. Error Trends Using Finite Difference Methods for y"+y=0, x=.5

Increment Size h	y(x) Exact	y(x) CFD	Error	y(x) FFD	Error
1/2	.569747	.571429	-.001682	.500000	.069747
1/4	.569747	.570156	-.000409	.533333	.036414
1/6	.569747	.569928	-.000181	.545455	.024292
1/8	.569747	.569849	-.000102	.551576	.018171
1/50	.569747	.569750	-.000003	——	——

Note from Table III, that as the interval spacing is halved, from $h=\frac{1}{2}$ to $h=\frac{1}{4}$, the error for the CFD method decreases on the order of $\frac{1}{4}$ or as h^2. For the FFD method, the error decreases on the order of h or approximately by $\frac{1}{2}$.

Times of Solution

The method of central finite differences was compared to the integral equation method for speed. The data from this analysis is contained in Table IV.

Table IV. Computer Time - y"+y=0

Method	Compilation Time (sec)	Execution Time (sec)	Usage (Kilo-word)
Integral Equation	0.735	1.178	199.410
CFD	0.531	0.546	166.875

The results of this comparison revealed that the CFD method required 53.6% less execution time, was compiled 27.8% faster, and used less storage than the integral equation method. The time savings can be attributed to the different coefficient matrices generated by each method. The CFD method gave a tridiagonal, sparse, 49 x 49 coefficient matrix. The integral method however resulted in a full, 50 x 50 coefficient matrix, which required more time and more manipulations to solve for the solution vector $y(x)$.

Accuracy

The central finite difference method was compared to the integral method for accuracy. Both methods were found to be equivalent; that is, the exact same solutions were obtained from both procedures, identical to 12 decimal places. Equivalency of the two methods was verified through matrix multiplication of equations (142) and (150). This was accomplished by rewriting, in corresponding matrix form, equation (147) and (152). The integral equation was expressed symbolically as

$$\bar{\bar{A}}\,\bar{x} = \bar{F} \tag{168}$$

where $\bar{\bar{A}}$ represents the coefficient matrix, $\bar{x}$ the solution vector, and $\bar{F}$ some function vector. The unknown $\bar{x}$, can be solved and is

$$\bar{x} = \bar{\bar{A}}^{-1}\bar{F} \tag{169}$$

where $\bar{\bar{A}}^{-1}$ is the matrix inverse of $\bar{\bar{A}}$. In a similar manner the CFD method, equation (150), was expressed symbolically as

$$\bar{\bar{B}}\bar{y} = \bar{R} \tag{170}$$

where $\bar{\bar{B}}$ represents the coefficient matrix associated with (121). The unknown $\bar{y}$, can be solved by matrix inversion and found to be

$$\bar{y} = \bar{\bar{B}}^{-1}\bar{R} \tag{171}$$

Since both methods yield identical solutions, that is

$$\bar{x} = \bar{y} \tag{172}$$

the expressions on the right side of equations (169) and (171) should also be equivalent, therefore

$$\bar{\bar{A}}^{-1}\bar{F} = \bar{\bar{B}}^{-1}\bar{R} \tag{173}$$

The necessary condition for equivalency is

$$\bar{F} = \bar{\bar{A}}\bar{\bar{B}}^{-1}\bar{R} \tag{174}$$

Equation (174) is easy to verify since $\bar{F}$ and $\bar{R}$ are already known and the coefficient matrices, $\bar{\bar{A}}$ and $\bar{\bar{B}}$, are internally generated. Using 7 iterations, equa-

tion (174) was verified by substituting the known quantities $\bar{\bar{A}}$, $\bar{\bar{B}}^{-1}$, and $\bar{R}$, the calculated $\bar{F}$ was found to be

$$\bar{F} = \begin{bmatrix} .142857 \\ .285713 \\ .428571 \\ .571428 \\ .714285 \\ .857143 \end{bmatrix} \tag{175}$$

The true value of $\bar{F}$, from the integral equation computer program, was

$$\bar{F} = \begin{bmatrix} .142857 \\ .285714 \\ .428571 \\ .571429 \\ .714286 \\ .857143 \end{bmatrix} \tag{176}$$

The reason for the discrepancy in the sixth decimal place pertains to a rounding error in the multiplication. The original computer program uses all 14 decimal places for internal computations. In this example only six significant figures were used and a rounding error results in the sixth decimal.

Conclusions

It was unforseen that both the CFD and integral approach would be identical. Though the two methods were solved using the methods of linear algebra each was characterized by a distinct different coefficient matrix, one being sparse for the CFD method, and the other being full for the integral approach. Both methods were shown to be of the same order of error,

h^2 . It is not possible to generalize at this point any other conclusions except that both methods are equivalent. The CFD solutions were noted to be computed faster in all circumstances but only because of the tridiagonal coefficient matrix. All computer solutions proved to be accurate with no significant round-off errors.

Case II

The second problem investigated was the one-dimensional inhomogeneous Helmholtz equation with homogeneous Dirichlet boundary conditions. Expressed mathematically, the problem is

$$\frac{d^2y(x)}{dx^2} + \lambda^2 y(x) = 1 \tag{177}$$

where $\lambda^2 = \frac{9\pi^2}{4}$, with boundary conditions

$$y(0) = 0, \qquad y(1) = 0 \tag{178}$$

Analytical Solution

As with all inhomogeneous 2nd order differential equations the solution can be expressed as a linear combination of solutions: homogeneous + particular. The complete general solution to (177) is

$$y(x) = A\cos\lambda x + B\sin\lambda x + \frac{1}{\lambda^2} \tag{179}$$

Using boundary conditions (178), the constants A and B

are evaluated, the unique solution is

$$y(x) = \frac{4}{9\pi^2}\left(\sin\frac{3\pi}{2}x - \cos\frac{3\pi}{2}x + 1\right) \tag{180}$$

and is graphed in Figure 10.

Integral Solution

The differential equation can be converted to integral form by first rearranging terms and solving for the second derivative. Equation (177) becomes

$$\frac{d^2y}{dx^2} = 1 - \lambda^2 y(x) \tag{181}$$

Integrate each side over the interval (o,x) to obtain

$$\frac{dy}{dx} = C + \int_0^x (1-\lambda^2 y(x))\,dx \tag{182}$$

where the constant C corresponds to $\frac{dy(0)}{dx}$. Integrate a second time over the same interval, equation (182) becomes

$$y(x) = Cx + \int_0^x\int_0^x (1-\lambda^2 y(x))\,dx\,dx \tag{183}$$

Using (6) on the double integration gives

$$y(x) = Cx + \int_0^x (x-\xi)(1-\lambda^2 y(x))\,d\xi \tag{184}$$

The constant C can now be evaluated by using the second boundary condition, $y(1)=0$:

$$y(1) = 0 = C + \int_0^1 (1-\xi)(1-\lambda^2 y(\xi))\,d\xi \tag{185}$$

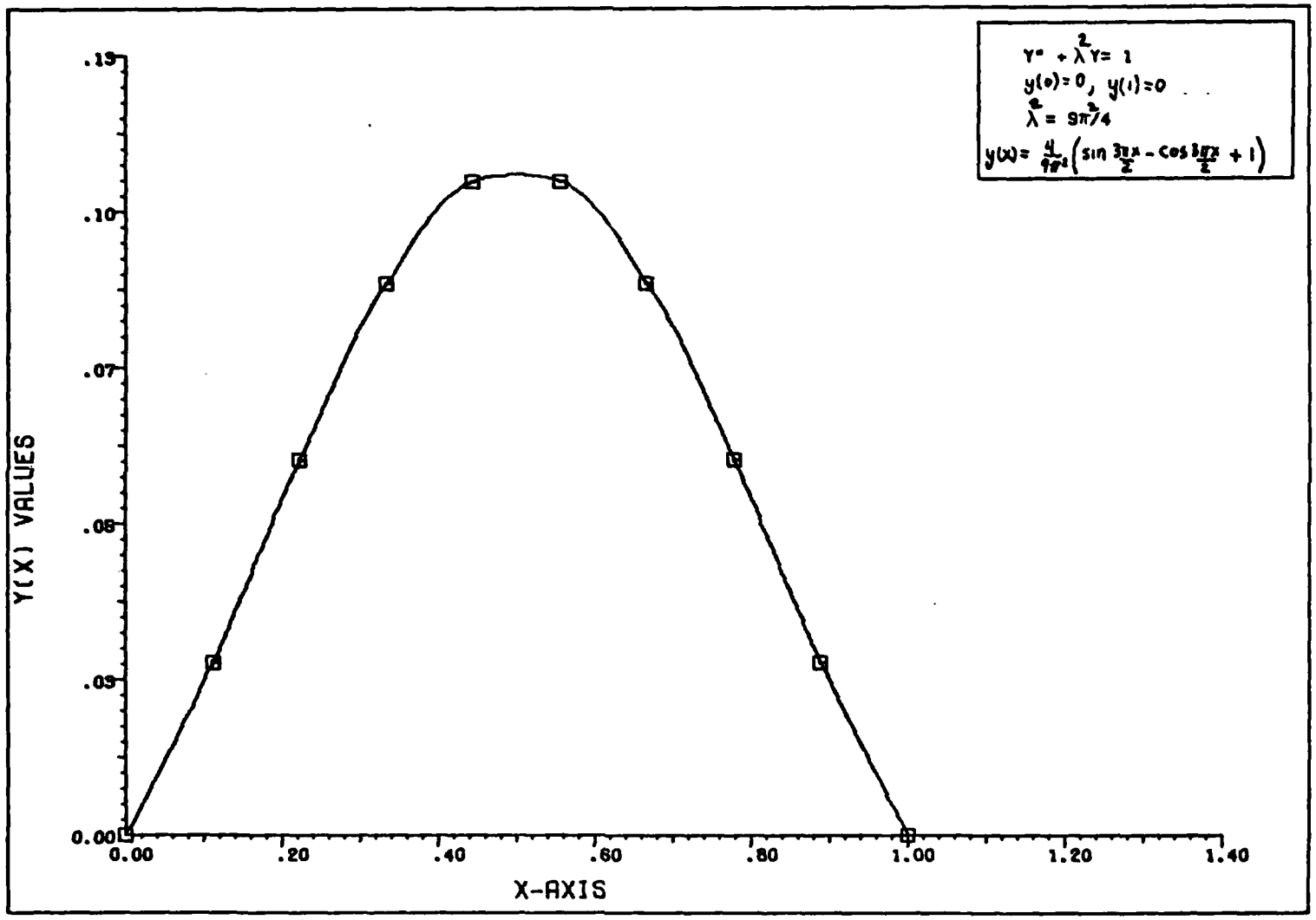

Fig. 10 Analytic Solution, Case II

Solving for C

$$C = \int_0^1 (1-\xi)(\lambda^2 y(\xi) - 1)\, d\xi \tag{186}$$

Substituting the expression for C into equation (184) yields

$$y(x) = \int_0^1 K(x,\xi)(\lambda^2 y(\xi) - 1)\, d\xi \tag{187}$$

with the kernel defined by the expression

$$K(x,\xi) = \begin{cases} x(1-\xi) & x < \xi \\ \xi(1-x) & x > \xi \end{cases} \tag{188}$$

Equation (187) represents the equivalent integral form for the one-dimensional Helmholtz equation.

Equation (187) can be rearranged by multiplying through by $K(x,\xi)$ and separating the integral. The integral equation containing y becomes

$$y(x) - \int_0^1 K(x,\xi)\lambda^2 y(\xi)\, d\xi = -\int_0^1 K(x,\xi)\, d\xi \tag{189}$$

The integral on the right simplifies by replacing $K(x,\xi)$ with its defined values over the appropriate limits of integration, that is

$$y(x) - \int_0^1 K(x,\xi)\lambda^2 y(\xi)\, d\xi =$$

$$-\left\{\int_0^x \xi(1-x)\, d\xi + \int_x^1 x(1-\xi)\, d\xi\right\} \tag{190}$$

Integrating out the ξ variable on the right side, equation (190) becomes

$$y(x) - \int_0^1 K(x,\xi)\lambda^2 y(\xi)d\xi = \frac{x}{2}(x-1) \tag{191}$$

The trapezoid approximation can now be used for the integral and equation (191) becomes equivalent to

$$y(x) - \sum_{k=1}^{N} D_k K(x,x_k)\lambda^2 y(x_k) = \frac{x}{2}(x-1) \tag{192}$$

Expressing D_k and $K(x,x_k)$ as matrices, equation (192) transforms into the system of linear equations

$$(\bar{\bar{I}} - \bar{\bar{D}}\bar{\bar{K}}\lambda^2)\bar{y} = \frac{\bar{x}}{2}(\bar{x}-1) \tag{193}$$

and is solved by the method of Gaussian elimination.

Green's Integral

In addition to the integral representation of equation (177) it is also possible to express the solution of $y(x)$ by the Green's integral, equation (27). From Appendix B , the Green's function for the Helmholtz operator was found to be

$$G(x,\xi) = \begin{cases} \dfrac{\sin\lambda(\ell-\xi)\sin\lambda x}{\lambda\sin\lambda\ell} & x < \xi \\[2ex] \dfrac{\sin\lambda(\ell-x)\sin\lambda\xi}{\lambda\sin\lambda\ell} & x > \xi \end{cases} \tag{194}$$

Therefore the equivalent expression for the Green's integral solution for $y(x)$ is

$$y(x) = -\int_0^1 G(x,\xi)\,d\xi \tag{195}$$

Using the trapezoid rule equation (195) becomes

$$y(x) = -\sum_{k=1}^{N} D_k G(x,x_k) \tag{196}$$

or, expressed in matrix notation

$$\bar{y} = -\bar{D}\,\bar{\bar{G}} \tag{197}$$

where $\bar{D}$ is the column vector of dimension Nx1 and $\bar{\bar{G}}$ the Green's matrix, defined by expression (194), of dimension NxN .

Finite Differences

The method of CFD was used to numerically differentiate equation (177). Substituting the central difference quotient, equation (97), for the second derivative and collecting common terms, equation (177) becomes

$$y_{i-1} - (2 - \lambda^2 h^2) y_i + y_{i+1} = h^2 \qquad i = 2,3,\ldots,N-1 \tag{198}$$

The equivalent matrix expression has the tridiagonal form

$$
\begin{bmatrix}
1 & -(2-\lambda^2h^2) & 1 & 0 & & & & \\
0 & 1 & -(2-\lambda^2h^2) & 1 & & & & \\
 & & & \cdot & & & & \\
 & & & & \cdot & & & \\
 & & & & & \cdot & & \\
 & & & 1 & -(2-\lambda^2h^2) & 1 & 0 \\
 & & & 0 & 1 & -(2-\lambda^2h^2) & 1
\end{bmatrix}
\begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_{N-1} \\ y_N \end{bmatrix}
= \begin{bmatrix} h^2 \\ h^2 \\ \vdots \\ h^2 \\ h^2 \end{bmatrix} \tag{199}
$$

Using the boundary conditions, $y_1 = 0$ and $y_N = 0$, expression (199) can be written in the form

$$
\begin{bmatrix}
-(2-\lambda^2h^2) & 1 & 0 & & & \\
1 & -(2-\lambda^2h^2) & 1 & & & \\
 & & \cdot & & & \\
 & & & \cdot & & \\
 & & & & \cdot & \\
 & & 1 & -(2-\lambda^2h^2) & 1 \\
 & & & 1 & -(2-\lambda^2h^2)
\end{bmatrix}
\begin{bmatrix} y_2 \\ y_3 \\ \vdots \\ y_{N-2} \\ y_{N-1} \end{bmatrix}
= \begin{bmatrix} h^2 \\ h^2 \\ \vdots \\ h^2 \\ h^2 \end{bmatrix} \tag{200}
$$

The dimensions of all three matrices have been reduced to N-2 . In more concise form equation (200) becomes

$$\bar{\bar{B}}\,\bar{y} = \bar{R} \tag{201}$$

where $\bar{\bar{B}}$ corresponds to the band coefficient matrix and $\bar{R}$ the function vector defined by the constant h^2 .

Relative Error

For a comparison of the relative errors associated with the three numerical methods based on the Helmholtz equation, see Figure 11. The relative error of the three numerical methods is shown in Table V. Once again identical results were obtained using the integral equation and CFD method

Table V. Relative Error (%) - Computer Solutions for $y''+\lambda^2 y=1$, $x=.5$

Number of Iterations per Interval	Integral-CFD Method	Green's Integral Method
2	35.253527	51.201617
4	7.609482	11.842646
6	3.472912	5.194057
8	1.971673	2.908348
50	0.051070	0.074035

Error Analysis

The same assumptions will be used for the error

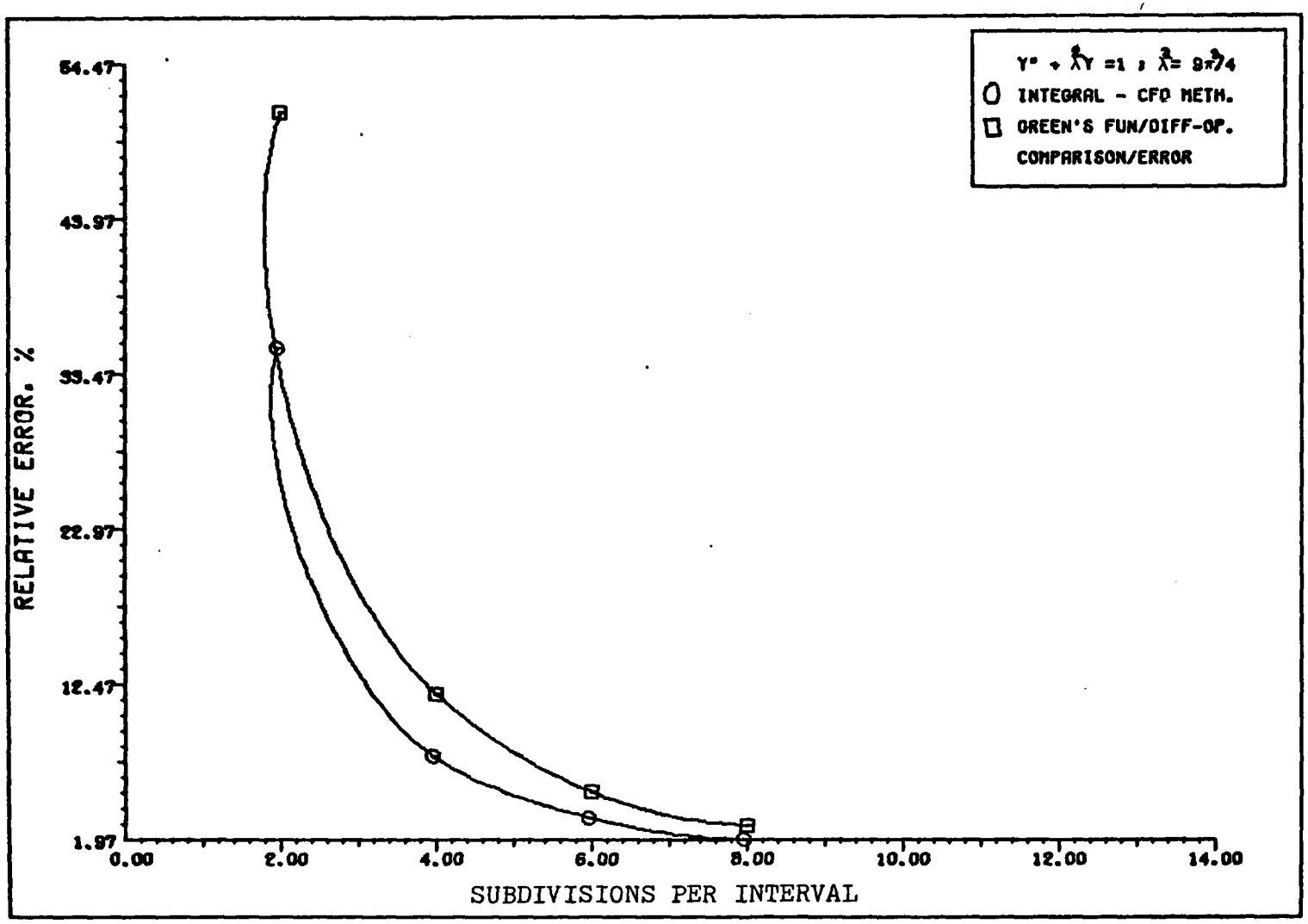

Fig. 11 Comparison of Relative Errors

analysis as were presumed in the first case study, all errors are strictly due to the method used and errors generated in the computational process could be neglected.

Integral Equation Errors

The integral equation, equation (187) and the Green's integral equation, equation (195), have both been shown to be equivalent; therefore, they should have associated with them the same order of error because the trapezoid rule is used to evaluate each integral. To predict the order of error the upper bound M must first be found. The Green's integral equation will be used for this analysis. Equation (195) can be written

$$y(x) = \int_0^x \frac{\sin \lambda(\ell - x) \sin \lambda \xi}{\lambda \sin \lambda \ell} \, d\xi + \int_x^1 \frac{\sin \lambda(\ell - \xi) \sin \lambda x}{\lambda \sin \lambda \ell} \, d\xi \tag{202}$$

where the expression for $G(x,\xi)$ has been used over its defined limits. The error will again be computed at the point $x = 1/2$, using the values $\lambda = \frac{3\pi}{2}$ and $\ell = 1$. Equation (202) becomes

$$y(x) = -.15 \left\{ \int_0^{1/2} \sin \frac{3\pi}{2} \xi \, d\xi + \int_{1/2}^1 \sin \frac{3\pi}{2}(1-\xi) \, d\xi \right\} \tag{203}$$

The total error of using expression (203) will be no greater than the sum of errors from each integral

$$f(\xi) = -.15 \left\{ \left| \sin \frac{3\pi}{2} \xi \right| + \left| \sin \frac{3\pi}{2}(1-\xi) \right| \right\} \tag{204}$$

Taking the first two derivatives of (204) and using the expression for the error bound, M is found to be

$$M \geq |f''(\xi)| = .15\left\{\frac{9\pi^2}{4}\sin\frac{3\pi\xi}{2} + \frac{9\pi^2}{4}\cos\frac{3\pi}{2}\xi\right\} \tag{205}$$

The maximum value for $\left\{\sin\frac{3\pi\xi}{2} + \cos\frac{3\pi}{2}\xi\right\}$ occurs when $\xi = \frac{\pi}{4}$, therefore the bound for M is

$$M = (.15)\frac{9\pi^2}{4}(1.3783) = 4.5911 \tag{206}$$

And the associated error is of the order

$$\text{Error} \cong \frac{(b-a)Mh^2}{12} = .3826\,h^2 \tag{207}$$

As h is decreased the associated error also decreases as a factor of h^2. This is observed in Table VI.

Table VI. Error Trends - Computer Solutions for $y''+\lambda^2 y=1$, $x=.5$

Increment Size, h	y(x) Exact	y(x) Cal Int-CFD	Error	y(x) Cal Green's	Error
1/2	.108716	.070390	.038326	.053052	.055664
1/4	.108716	.100443	.008273	.095841	.012875
1/6	.108716	.104940	.003776	.103069	.005647
1/8	.108716	.106572	.002144	.105554	.003162
1/50	.108716	.108660	.000056	.108635	.000081

In addition to the above table the relative error was examined at each array element when the interval (0,1) was subdivided into 50 partitions. Because the integral

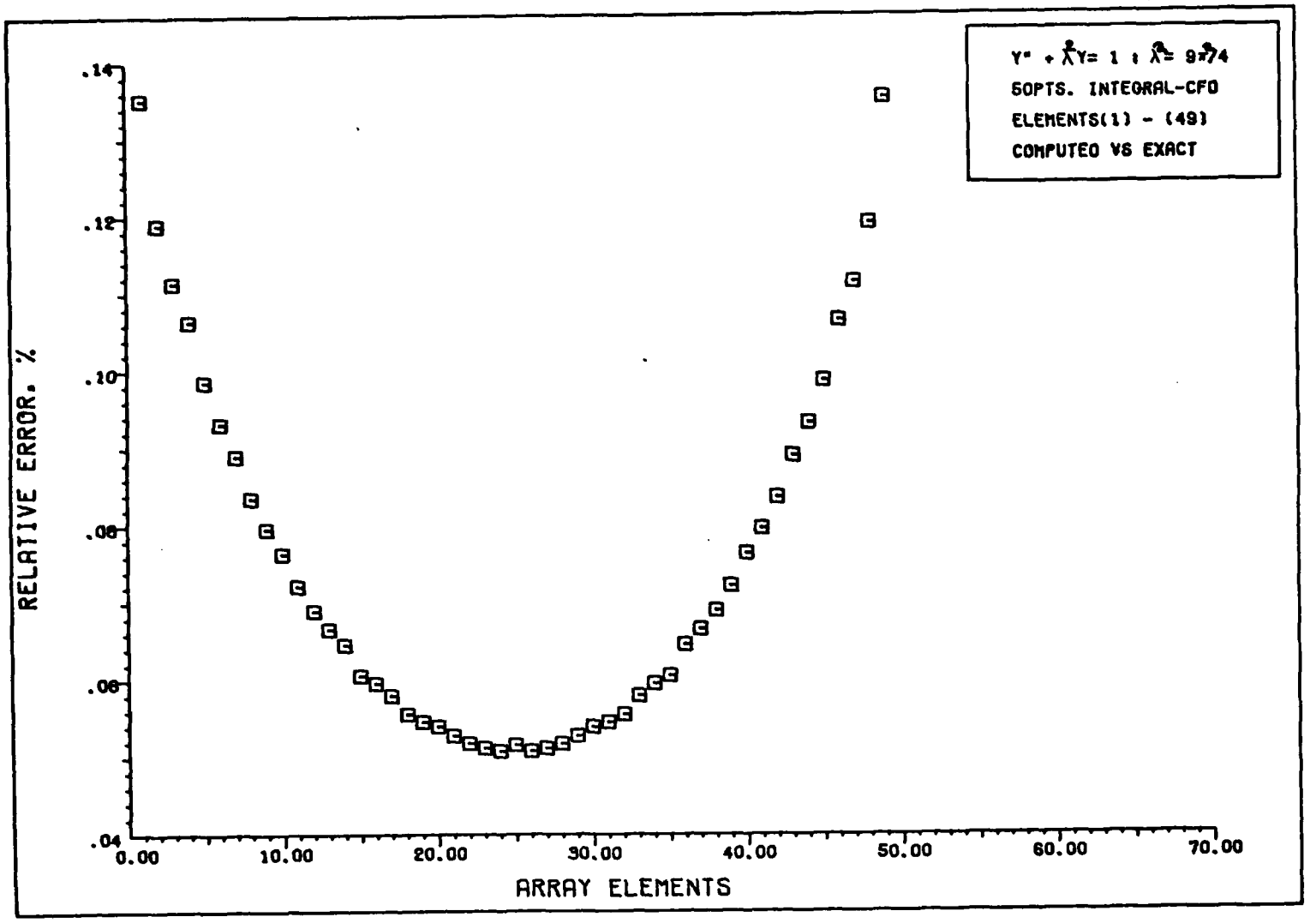

Fig. 12 Relative Errors of Array Elements
Integral - CFD Methods

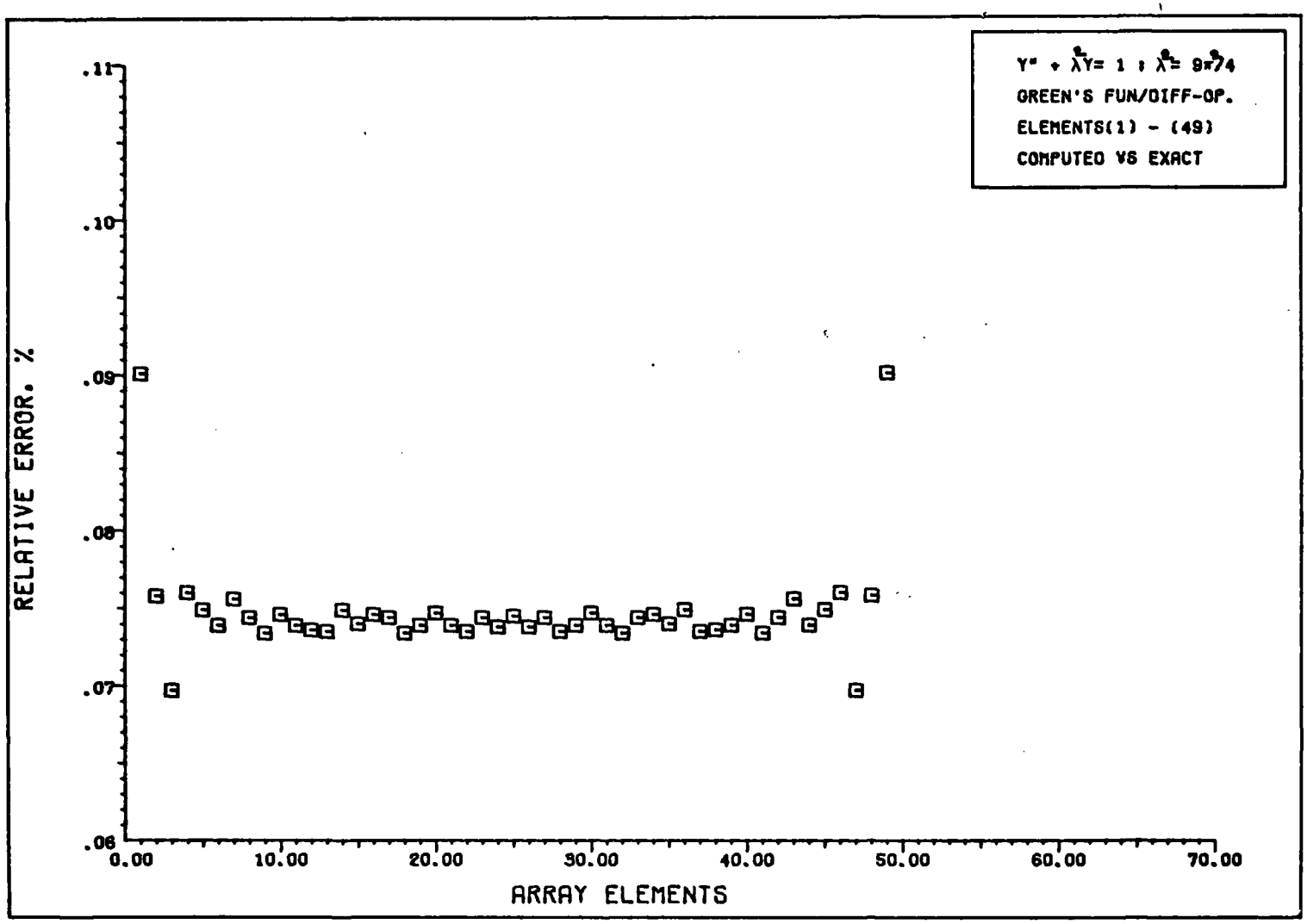

Fig. 13 Relative Errors of Array Elements
Green's Integral Equation

and CFD methods gave identical results their errors both appear in Figure 12. The Green's integral was also analyzed at each array element and appears in Figure 13. It can be seen from both sets of dats that the errors are symmetric and largest in the neighborhoods of the end points. This is attributed to the functional form of both $y(x)$ and the Green's function. At the end points the two functions have their steepest incline therefore larger errors are introduced over the same size increments across these regions. At those points along the center of the interval, where the functions change more slowly, less error in the increment is introduced. Note that the Green's integral method is more accurate at the outer elements (1) - (10) and (40) - (49). The integral - CFD method is more accurate at the inner elements (11) - (39). Also the error trend in the Green's method is averaged out to almost a constant .075% while the CFD - integral method appears parabolic across the region.

Finite Differences Errors

No additional error analysis was carried out for the method of finite differences. It was noted that errors associated with the CFD method once again were of order h^2 due to the second order truncation in the Taylor series expansion for $y(x)$.

Times of Solution

The two numerical untegration routines were compared to the CFD method for speed and storage. The interval (0,1) was divided into 50 partitions, resulting in a set of 49 linear equations for the CFD method and a set of 51 linear equations for the integral method. Using the Green's integral expression the solution was obtained by matrix multiplication. The data for these three methods are contained in Table VII.

Table VII. Computer Time - $y'' + \lambda^2 y = 1$

Method	Compilation Time (sec)	Execution Time (sec)	Usage (Kilo-word)
Integral Equation	.784	1.177	194.460
Green's Integral	.600	0.441	116.319
CFD	.548	0.558	170.556

The CFD method was 2.1 times faster than the integral equation method. In addition, it was compiled in 30.1% less time and used 12.3% less central storage. The Green's integral method was found to be quickest and used the least amount of storage.

Conclusions

The CFD and integral equation methods both proved

to be identical. Though the two were again charcterized by distinct coefficient matrices, they were found to be equivalent. A second integral approach was analyzed by solving for the exact Green's function based upon the Helmholtz operator. Solutions of this integral equation proved to be, on the average, of the same order of magnitude as the CFD - integral methods but resulted in a smoother error curve over the calculated values. Also the Green's integral calculations proved quicker than either the integral equation method or using the CFD quotient.

Case III

The third and final problem investigated in one-dimension was the inhomogeneous Cauchy-equation with homogeneous Dirichlet boundary conditions. Expressed mathematically, the problem is

$$x^2 \frac{d^2y}{dx^2} - 2y = x^4 \tag{208}$$

with boundary conditions

$$y(1) = 0, \qquad y(3) = 0 \tag{209}$$

Both previous results, that is, converting the differential equation into integral form and approximating the solution through numerical integration and using the method of finite differences have proven to be equivalent. One possible reason for this could

be due to the linear kernel which has resulted in both integral conversions. Equation (208) was found not to have a linear kernel upon integral conversion. The properties of this equation are now investigated.

Analytical Solution

The complete general solution to (208) is found to be

$$y(x) = \frac{A}{x} + Bx^2 + \frac{x^4}{10} \tag{210}$$

Using boundary conditions (209), the constants A and B are evaluated. The unique solution is

$$y(x) = \left(\frac{108}{130}\right)\frac{1}{x} - \left(\frac{121}{130}\right)x^2 + \frac{x^4}{10} \tag{211}$$

and is graphed in Figure 14. Note that the solution is asymmetric.

Integral Solution

The Cauchy differential equation can be expressed in integral form by first rearranging terms and solving for the second derivative. Equation (208) becomes

$$\frac{d^2y(x)}{dx^2} = x^2 - \frac{2y(x)}{x^2} \tag{212}$$

Now, integrate both sides with respect to x over the interval (1,x). Equation (212) becomes

$$\frac{dy(x)}{dx} = C + \int_1^x \left(x^2 - \frac{2y(x)}{x^2}\right) dx \tag{213}$$

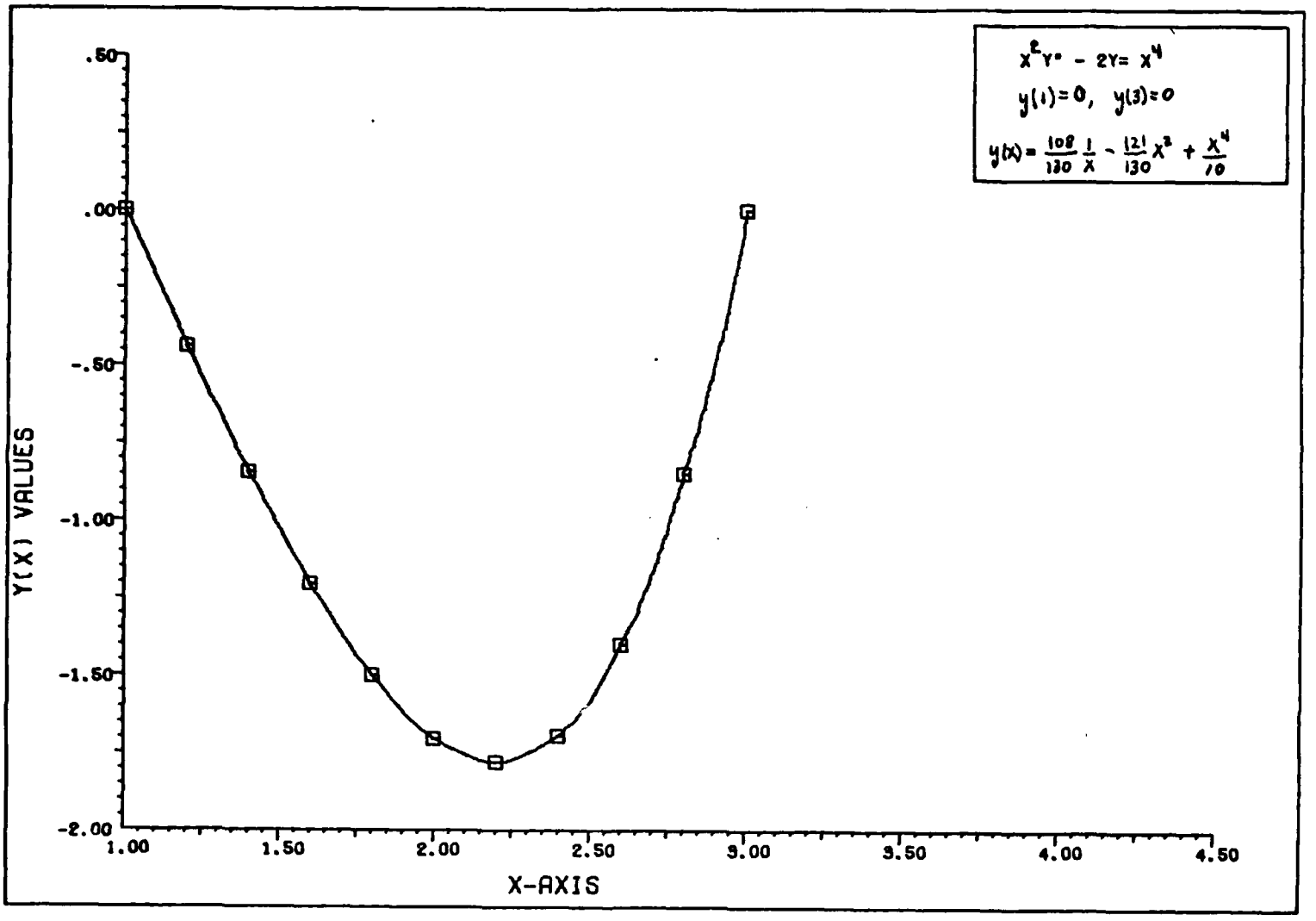

Fig. 14 Analytic Solution, Case III

where the constant C represents $\frac{dy(0)}{dx}$. Integrating a second time over the same limits makes (213) equivalent to

$$y(x) = C\int_1^x dx + \int_1^x\int_1^x \left(x^2 - \frac{2y(x)}{x^2}\right) dx \tag{214}$$

By using the results of (6) for the multiple integral and performing the integration of the first integral, equation (214) becomes

$$y(x) = Cx - C + \int_1^x (x-\xi)\left\{\xi^2 + \frac{2y(\xi)}{\xi^2}\right\} d\xi \tag{215}$$

The constant C can be evaluated by using the boundary condition $y(3) = 0$.

$$y(3) = 0 = 2C + \int_1^3 (3-\xi)\left\{\xi^2 + \frac{2y(\xi)}{\xi^2}\right\} d\xi \tag{216}$$

Solving for C yields:

$$C = \frac{1}{2}\int_1^3 (\xi-3)\left\{\xi^2 + \frac{2y(\xi)}{\xi^2}\right\} d\xi \tag{217}$$

Using this expression for C, the complete solution for $y(x)$, given by equation (215) becomes

$$y(x) = \int_1^3 (x-\xi)\left\{\xi^2 + \frac{2y(\xi)}{\xi^2}\right\} d\xi + \frac{(x-1)}{2}\int_1^3 (\xi-3)\left\{\xi^2 + \frac{2y(\xi)}{\xi^2}\right\} d\xi \tag{218}$$

Equation (218) can be put in the simplified form

$$y(x) = \int_1^3 K(x,\xi)\left\{\xi^2 + \frac{2y(\xi)}{\xi^2}\right\} d\xi \tag{219}$$

by using the abbreviation

AD-A080 415 AIR FORCE INST OF TECH WRIGHT-PATTERSON AFB OH SCHOO--ETC F/G 12/1
NUMERICAL METHODS AND THE SOLUTION OF BOUNDARY VALUE PROBLEMS.(U)
DEC 79 G N NELSON
UNCLASSIFIED AFIT/GEP/PH/79D-7 NL

2 OF 2
AD
A080415

END
DATE
FILMED
3-80
DDC

$$K(x,\xi) = \begin{cases} \dfrac{(x-1)(\xi-3)}{2} \\ \dfrac{(x-3)(\xi-1)}{2} \end{cases} \tag{220}$$

Equation (219) represents the equivalent integral form of the one-dimensional Cauchy equation. The integral equation can be rearranged by multiplying through by and seperating tne integral. Combining terms, equation (219) is also equivalent to the expression

$$y(x) - 2\int_1^3 \frac{K(x,\xi)\,y(\xi)}{\xi^2}\,d\xi = \int_1^3 K(x,\xi)\,\xi^2\,d\xi \tag{221}$$

The integral on the right simplifies by replacing the kernel with its values over the appropriate limits. The integral becomes

$$\int_1^x \frac{(x-3)(\xi-1)\,\xi^2}{2}\,d\xi + \int_x^3 \frac{(x-1)(\xi-3)\,\xi^2}{2}\,d\xi \tag{222}$$

Integrating both integrals over ξ, equation (222) becomes

$$\frac{x^4}{12} - \frac{10}{3}x + \frac{13}{4} \tag{223}$$

Equation (221) then becomes

$$y(x) - 2\int_1^3 \frac{K(x,\xi)\,y(\xi)}{\xi^2}\,d\xi = \frac{x^4}{12} - \frac{10}{3}x + \frac{13}{4} \tag{224}$$

It is now possible to use the trapezoid approximation for the left side integral and equation (224) becomes

$$y(x) - 2\sum_{k=1}^{N} \frac{D_k K(x,x_k)\, y(x_k)}{x_k^2} = \frac{x^4}{12} + \frac{10}{3}x + \frac{13}{4} \qquad (225)$$

where the points $\xi = x_k$ have been chosen over the interval (1,3). In matrix notation expression (225) transforms into the system of linear equations

$$\left\{ \bar{\bar{I}} - \bar{\bar{D}}\,\bar{\bar{K}}' \right\} \bar{y} = \bar{x} \qquad (226)$$

where $\bar{\bar{D}}$ corresponds to the weighing coefficients used in the numerical integration, $\bar{\bar{K}}'$ is the modified kernel $K(x,x_k)$ with x_k^2 denominator, and $\bar{x}$ corresponds to the function vector defined by (223). Equation (226) can now be solved using Gaussian elimination.

Green's Integral

In addition to the integral representation it is also possible to express the solution of $y(x)$ by the Green's integral equation. From Appendix C, the Green's function for the one-dimensional Cauchy operator was found to be

$$G(x,\xi) = \begin{cases} \frac{27}{18}\left(\frac{\xi^2}{27} - \frac{1}{\xi}\right)\left(\frac{1}{x} - x^2\right) & x < \xi \\ \frac{27}{18}\left(\xi^2 - \frac{1}{\xi}\right)\left(\frac{1}{x} - \frac{x^2}{27}\right) & x > \xi \end{cases} \qquad (227)$$

Therefore the equivalent expression for $y(x)$ can be expressed as

$$y(x) = -\int_{1}^{3} G(x,\xi)\,\xi^2\,d\xi \tag{228}$$

where $G(x,\xi)$ is as defined above. Using the trapezoid rule, equation (228) becomes equivalent to the quantity

$$y(x) \cong -\sum_{K=1}^{N} D_K\, G(x,x_K)\, x_K^2 \tag{229}$$

or in matrix notation $y(x)$ appears as

$$y(x) = -\bar{\bar{D}}\,\bar{\bar{G}}\,\bar{x}^2 \tag{230}$$

where $\bar{\bar{D}}$ and $\bar{\bar{G}}$ are both matrix vectors of dimension N X N and $\bar{x}^2$ is the column vector of dimension N X 1.

Finite Differences

The method of finite differences was used to compare numerical differentiation with the integral and Green's methods outlined above. Again, the derived central finite difference quotient, equation (97), was substituted into the one-dimensional Cauchy equation. After collecting terms, equation (208) became equivalent to the expression

$$y_{i-1} - \left(2 + \frac{2h^2}{x_i^2}\right) y_i + y_{i+1} = x_i^2 h^2 \tag{231}$$

The matrix has the tridiagonal form

$$
\begin{bmatrix}
1 & -\left(2+\frac{2h^2}{x_2^2}\right) & 1 & 0 & & & \\
0 & 1 & -\left(2+\frac{2h^2}{x_3^2}\right) & 1 & & & \\
 & & \ddots & \ddots & \ddots & & \\
 & & & 1 & -\left(2+\frac{2h^2}{x_{N-2}^2}\right) & 1 & 0 \\
 & & & 0 & 1 & -\left(2+\frac{2h^2}{x_{N-1}^2}\right) & 1
\end{bmatrix}
\begin{bmatrix}
y_1 \\ y_2 \\ \vdots \\ y_{N-2} \\ y_{N-1}
\end{bmatrix}
=
\begin{bmatrix}
x_2^2 h \\ x_3^2 h \\ \vdots \\ x_{N-2}^2 h \\ x_{N-1}^2 h
\end{bmatrix}
\tag{232}
$$

Using the boundary conditions, $y_1 = 0$ and $y_N = 0$, expression (232) can be rewritten in the form

$$
\begin{bmatrix}
-\left(2+\frac{2h^2}{x_2^2}\right) & 1 & 0 & & & \\
1 & -\left(2+\frac{2h^2}{x_3^2}\right) & 1 & & & \\
 & & \ddots & \ddots & \ddots & \\
 & & 1 & -\left(2+\frac{2h^2}{x_{N-2}^2}\right) & 1 \\
 & & & 1 & -\left(2+\frac{2h^2}{x_{N-1}^2}\right)
\end{bmatrix}
\begin{bmatrix}
y_2 \\ y_3 \\ \vdots \\ y_{N-3} \\ y_{N-2}
\end{bmatrix}
=
\begin{bmatrix}
x_3^2 h^2 \\ x_4^2 h^2 \\ \vdots \\ x_{N-3}^2 h^2 \\ x_{N-2}^2 h^2
\end{bmatrix}
\tag{233}
$$

The dimensions of all three matrices have been reduced to N - 2. In concise matrix form expression (233) can be written

$$\bar{\bar{B}}\bar{y} = \bar{R} \tag{234}$$

where $\bar{\bar{B}}$ corresponds to the given band coefficient matrix and $\bar{R}$ represents the column function vector defined by the right-hand quantity in (233).

Relative Error

For a comparison of the relative errors associated with the three numerical methods see Figure 15. The relative error percentages are tabulated in Table VIII.

Table VIII. Relative Error (%) - Computer Solution for $x^4y''-2y=x^4, x=2$

Number of Iterations per Interval	Integral Equation	Green's Integral Method	CFD Method
2	2.402402	.150144	6.306306
4	.732556	.009369	1.718748
6	.344530	.001815	.784274
8	.198287	.000586	.445971
50	.005241	.000000	.011593

Error Analysis

Because both the integral and Green's representations are equivalent either expression can be used to predict an error bound using the trapezoid rule. The

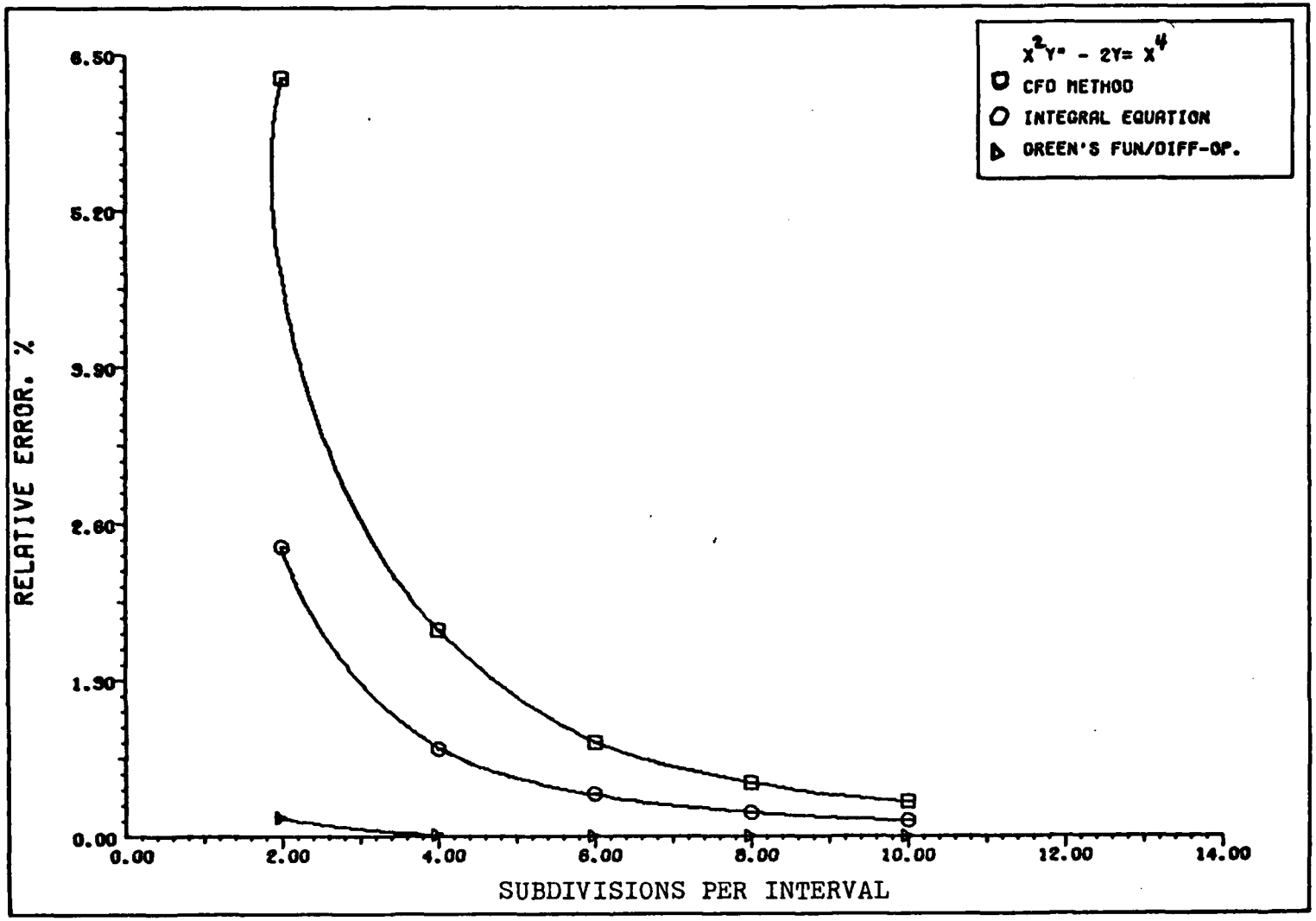

Fig. 15 Comparison of Relative Errors

Green's integral representation is used once again because it does not involve the function $y(\xi)$, making the error calculations easier to work with. The Green's integral, equation (228), can be written

$$y(x) = -\left\{ \int_1^x \frac{27}{78}\left(\xi^2 - \frac{1}{\xi}\right)\left(\frac{1}{x} - \frac{x^2}{27}\right)\xi^2 \, d\xi \right.$$

$$\left. + \int_x^3 \frac{27}{78}\left(\frac{\xi^2}{27} - \frac{1}{\xi}\right)\left(\frac{1}{x} - x^2\right)\xi^2 \, d\xi \right\} \tag{235}$$

where $G(x,\xi)$ has been substituted over the appropriate limits. The error will be computed at the point $x = 2$ and expression (235) simplifies to

$$y(x) = -\left\{ .1218 \int_1^2 (\xi^4 - \xi)\, d\xi - 1.2115 \int_2^3 \left(\frac{\xi^4}{27} - \xi\right) d\xi \right\} \tag{236}$$

The maximum error for both integrals is the sum of errors associated from each. To find the upper bound on the errors all errors are assumed to be additive. The upper bound M can now be associated with $f(\xi)$, where $f(\xi)$ corresponds to the sum of the two integrands above:

$$f(\xi) = .1218(\xi^4 - \xi) + 1.2115\left(\frac{\xi^4}{27} - \xi\right) \tag{237}$$

To calculate M the second derivative of $f(\xi)$ is needed. This is given by

$$f''(\xi) = 1.4616\,\xi^2 + .5484\,\xi^2 = 2\xi^2 \tag{238}$$

The value of $f''(\xi)$ at the point $\xi = 2$ is found to be

Table IX. Error Trends - Computer Solutions for $x^2y''-2y=x^4$, $x=2$

Increment Size, h	y(x) Exact	y(x) Integral	Error	y(x) Green's	Error	y(x) CFD	Error	Calculated Error
1	-1.707692	-1.666667	.041025	-1.705028	.002664	-1.600000	.107692	.666667
1/2	-1.707692	-1.695187	.012505	-1.707532	.000160	-1.678341	.029351	.166675
1/3	-1.707692	-1.701809	.005883	-1.707661	.000031	-1.694299	.013393	.074074
1/4	-1.707692	-1.704306	.003386	-1.707682	.000010	-1.700076	.007616	.041667
1/5	-1.707692	-1.705501	.002191	-1.707688	.000004	-1.702792	.004900	.026667
1/25	-1.707692	-1.707603	.000089	-1.707692	.000000	-1.707494	.000198	.001067

$$M \geq |f''(\xi)| = 4 \tag{239}$$

and the associated error is of the order

$$\text{Error} \cong \frac{(b-a)Mh^2}{12} = .6667\ h^2 \tag{240}$$

This error represents only a crude approximation to those errors associated using trapezoid integration and can be misleading. All errors in arriving at (240) were assumed to be additive. Because many of these errors cancel the predicted values will always be larger than observed, as seen in Table IX.

The relative error was also examined at each array element when the interval (1,3) was divided into 50 partitions. The errors associated with the integral solution are graphed in Figure 16. The Green's integral solution converged to the exact solution at every array point, to six decimal place accuracy and was not graphed. The relative error associated with the CFD method was also examined at each array element and is graphed in Figure 17. Note that both sets of data display similar trends; the higher numbered array elements have lower errors as compared to the lower numbered array elements. This trend can be explained by examining the method of solution. Both methods require the simultaneous solution of a set of N algebraic equations, 49 equations for the CFD method and

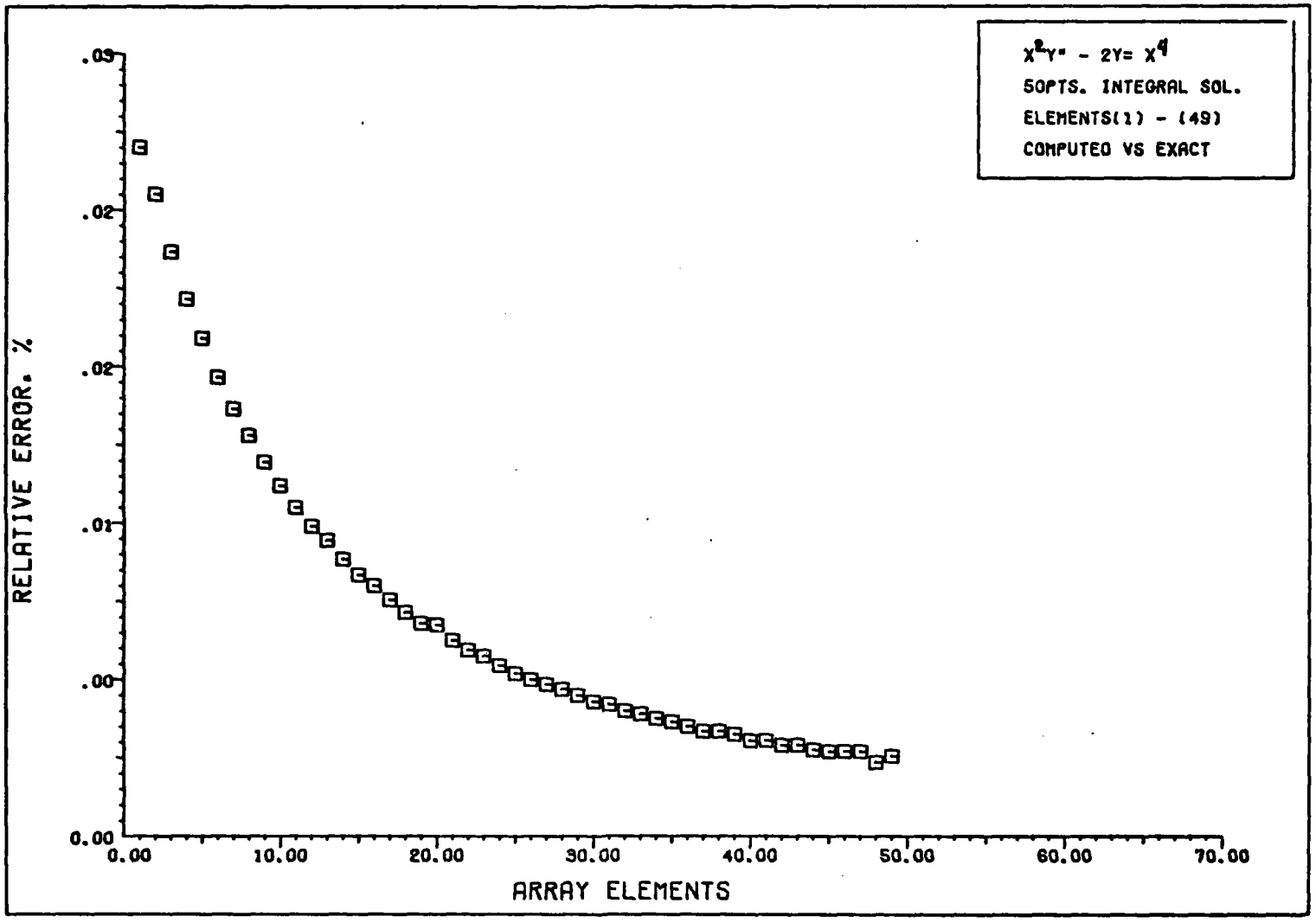

Fig. 16 Relative Errors of Array elements
Integral Equation Method

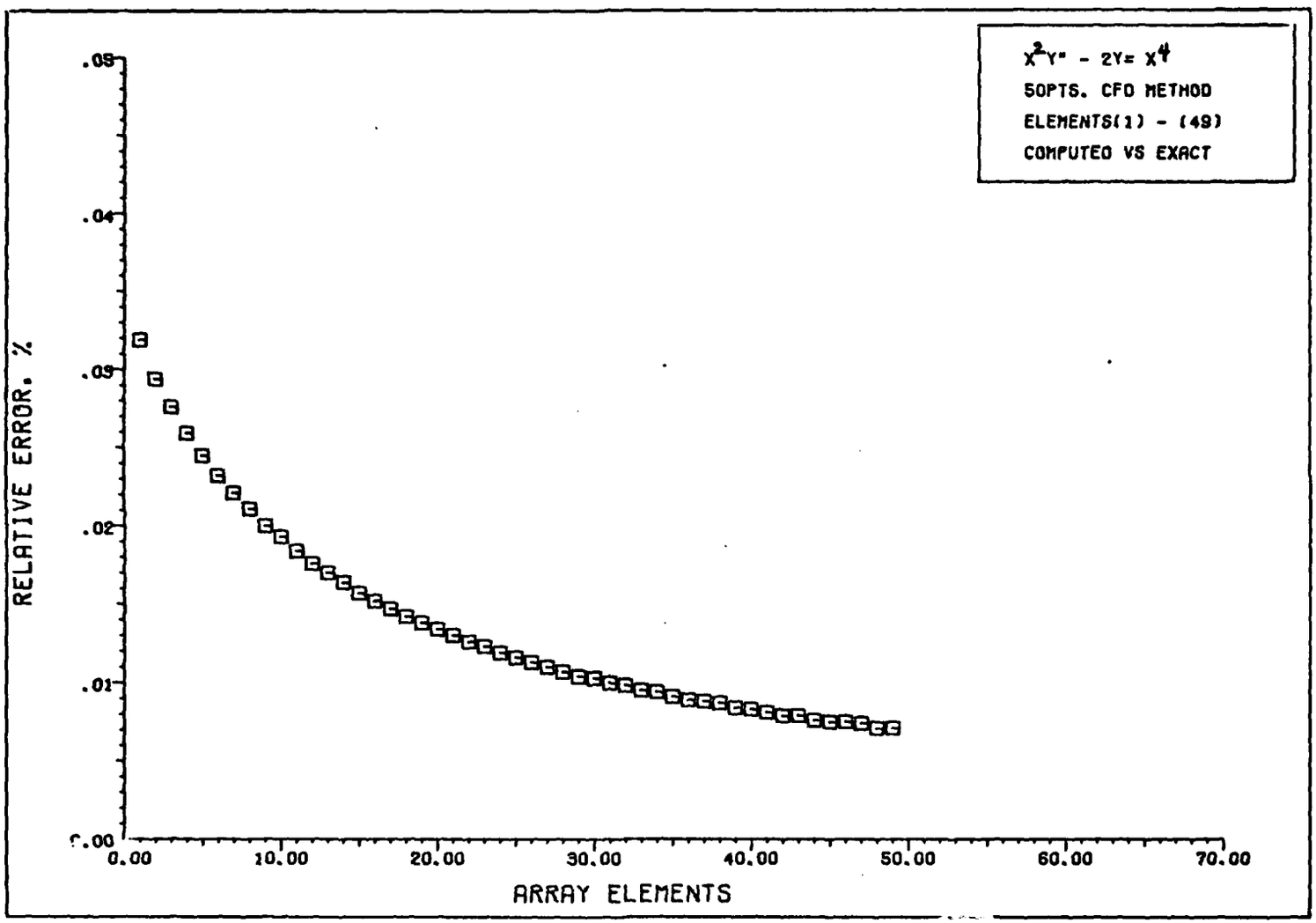

Fig. 17 Relative Errors of Array Elements - CFD Method

51 for the integral approach. Both sets are solved by Gaussian elimination. As was covered earlier the last array elements are evaluated first and therefore have the smallest round-off errors. As the elements above are computed from the know elements below there is an accumulation of air with each new row evaluated. This accounts for the trend in increasing error as the last elements are calculated, corresponding to the lower numbered array elements.

Simpson's Comparison

The trapezoid rule was compared to the Simpson's rule for the same array elements as above, see Figures 18 and 19. Note the downward trend for the relative error values at the higher indexed array elements in both figures. Also, the same sinusoidal character is exhibited over the odd - even partitions as was observed in Figure 8. In addition, Simpson's rule gives a better approximation to the calculated values at the odd numbered intervals than the trapezoid rule. This results because the kernel associated with the integral equation is no longer a linear function, but rather can be expressed as the modified kernel

$$K'(x,\xi) = \begin{cases} \dfrac{(x-1)(\xi-3)}{2\xi^2} & x < \xi \\ \dfrac{(x-3)(\xi-1)}{2\xi^2} & x > \xi \end{cases} \tag{241}$$

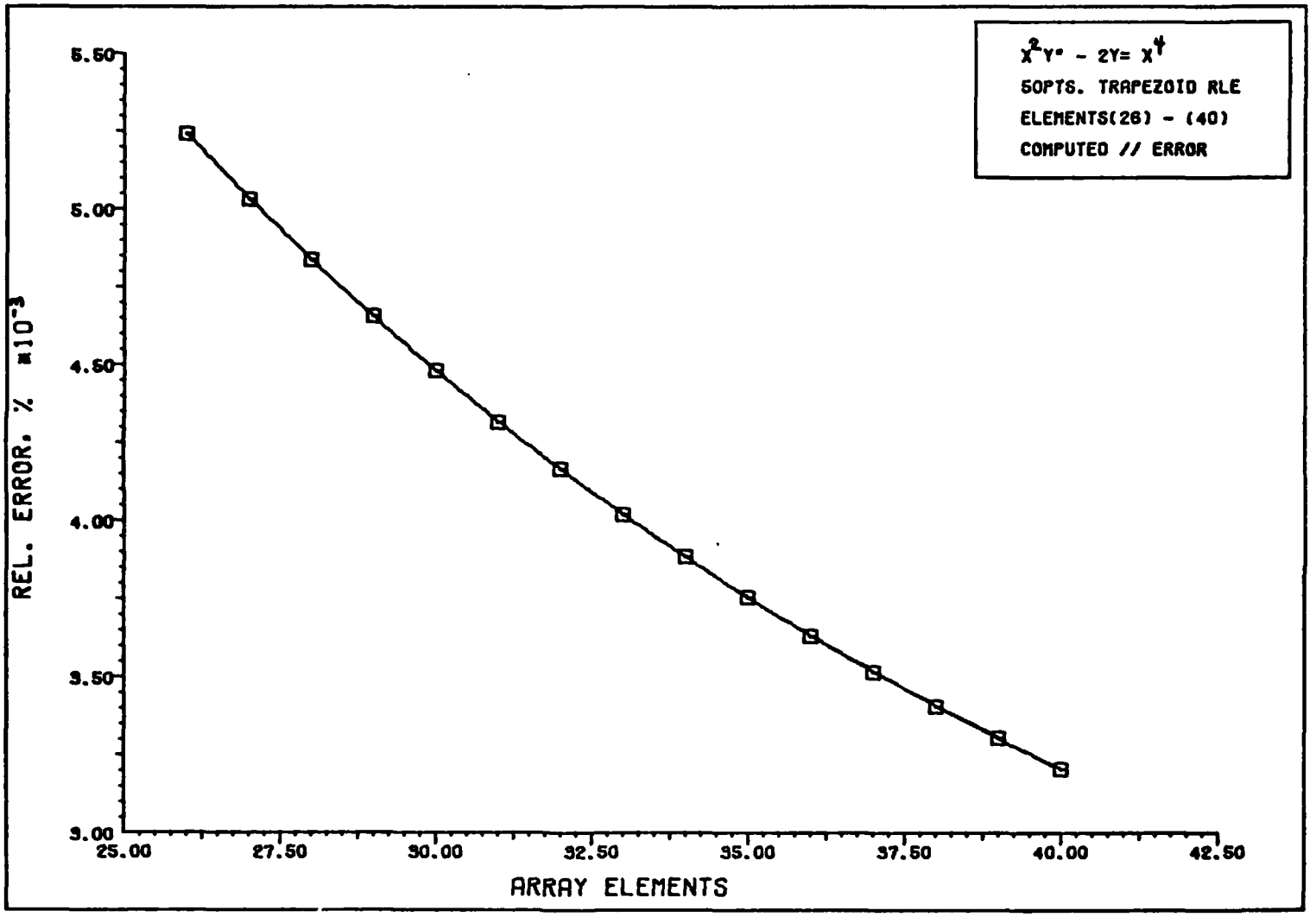

Fig. 18 Relative Errors Using Trapezoid Rule

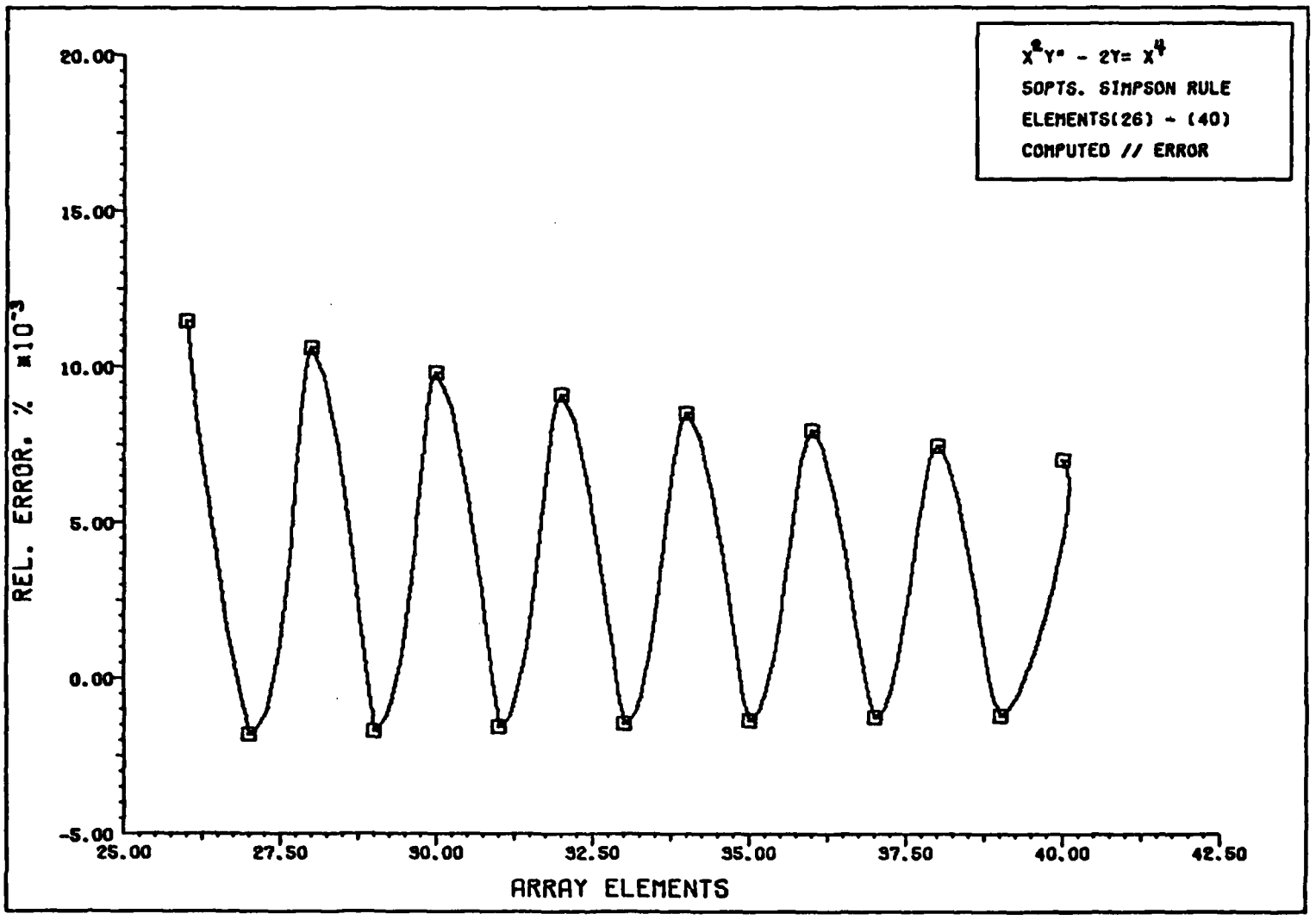

Fig. 19 Relative Errors Using Simpson's Rule

Quadratic interpolation, i.e., parabolas, provide a more accurate estimate of the non-linear kernel than using trapezoids.

Times of Solution

The two numerical integration routines were compared to the CFD method for speed. The results of this comparison are given in Table X.

Table X. Computer Time - $x^2 y''-2y=x^4$

Method	Compilation Time (sec)	Execution Time (sec)	Usage (Kilo-word sec)
Integral Equation	0.799	1.186	194.087
Green's Integral	0.662	0.847	117.473
CFD	0.566	0.557	169.940

The CFD method was executed 2.1 times faster than the integral equation method and 1.5 times as fast as the Green's integral approach. In addition, the CFD method was compiled 29.2% faster and used 12.4% less central storage than the integral method. Also, the CFD method was complied 14.5% faster and used 30.8% more central storage compared to the Green's integral equation.

Conclusions

The one significant feature about the one-dimen-

sional Cauchy-type equation is the fact that its solution is asymmetric. Converting the original differential equation into integral form still results in a linear weighted Green's kernel but multiplied by a non-linear function of ξ . Also the Green's integral equation, for the differential operator, has a non-symmetric Green's kernel. Results by the Green's integral equation proved superior to the other two methods. The integral equation method also gave more accurate solutions as compared to the CFD method.

IV. Two Dimensional Numerical Methods

The Steady-State Heat Conduction Problem

The last case investigated in this thesis will be the two-dimensional steady-state heat conduction problem with inhomogeneous Dirichlet boundary conditions. The internal temperature within the rectangular plate, shown in Figure 20, staisfies the partial differential equation

$$\nabla^2 T(x,y) = -F(x,y) \tag{242}$$

where $T(x,y)$ is the temperature at the point (x,y) and $F(x,y)$ represents the internal heat generation.

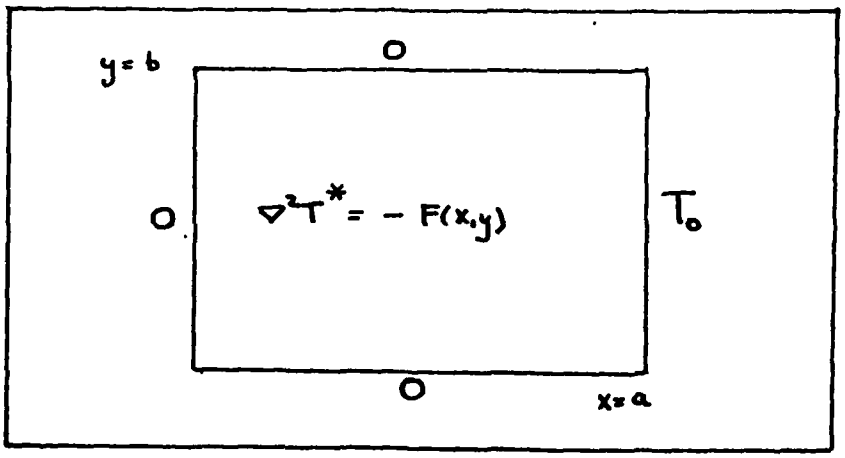

Fig. 20 Two-Dimensional Steady-State Heat Conduction Problem

The boundary conditions, from Figure 20 are

$$T(x,0) = T(0,y) = T(x,b) = 0, \quad T(a,y) = T_0 \tag{243}$$

where T_o represents some constant temperature along the edge $x = a$. For all problems considered, $F(x,y)$ is assumed constant over the plate and has the value

$$F(x,y) = 1 \tag{244}$$

Analytical Solution

The analytical closed-form solution of equation (242), Poisson's equation, can be expressed as the sum of the two harmonic functions; the first satisfies equation (242) with homogeneous Dirichlet boundary conditions, and the second function satisfies the Laplacian of (242) with the inhomogeneous boundary condition at $T(a,y)$. The complete solution, using condition (243) and satisfying the given boundary conditions, is derived in Appendix D and found to be

$$T(x,y) = -\frac{16a^2b^2}{\pi^4}\sum_{n=1}^{\infty}\sum_{m=1}^{\infty}\frac{1}{nm(a^2m^2+b^2n^2)}\sin\frac{n\pi x}{a}\sin\frac{m\pi y}{b}$$

$$+\frac{4T_o}{\pi}\sum_{n=1}^{\infty}\frac{1}{n}\left(\sinh\frac{n\pi}{b}x\sin\frac{n\pi y}{b}\right)\Big/\left(\sinh\frac{n\pi a}{b}\right) \tag{245}$$

Note that the solution is a double Fourier series, a summation process which, if slowly convergent will take considerable time. For the problem under investigation the temperature at 16 interior nodal points was examined. Also, instead of using the rectangular area the analytical model was altered into a square

of unit dimension. From equation (245) the internal temperature was computed at 81 interior grid points, a computation requiring 70.9 seconds for six place decimal accuracy.

Finite Differences

The solution to the two-dimensional steady-state heat conduction problem by finite difference methods is simply an extension of the technique used in the one-dimensional cases. The first step is to set up a grid system of interior points within the plate, shown in Figure 21.

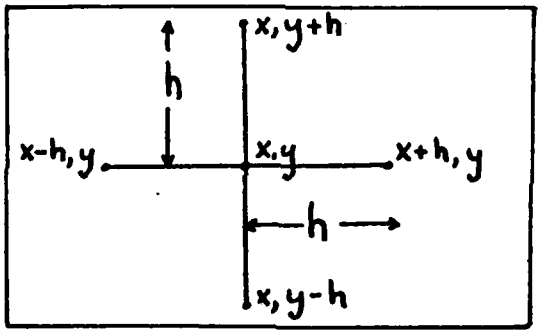

Fig. 21 Interior Grid Network

The Laplacian of equation (242) can be approximated by expressing the two second derivatives of the temperature as a difference equation. The second derivatives, using equation (97) and the interior nodal system in Figure 21 become

$$\frac{d^2T(x,y)}{dx^2} = \frac{T(x-h,y) - 2T(x,y) + T(x+h,y)}{h^2} \tag{246}$$

and

$$\frac{d^2T(x,y)}{dy^2} = \frac{T(x,y-h) - 2T(x,y) + T(x,y+h)}{h^2} \tag{247}$$

Substituting these approximations back into the heat equation,(242), and the combining terms gives the expression

$$T(x-h,y) + T(x+h,y) - 4T(x,y)$$

$$+ T(x,y-h) + T(x,y+h) = -F(x,y)h^2 \tag{248}$$

Once again the finite difference method results in a set of linear algebraic equations.

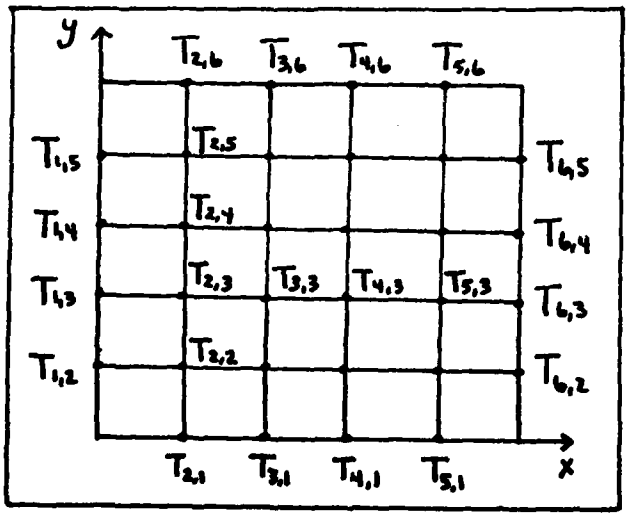

Fig. 22 Interior Nodal Arrangement

Using the nodal point coordinate system, shown in Figure 22, and the boundary conditions given by expression (243), the following matrix representation of equation (248) is obtained

$$
\begin{bmatrix}
-4 & 1 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
1 & -4 & 1 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 1 & -4 & 1 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 1 & -4 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
1 & 0 & 0 & 0 & -4 & 1 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 1 & 0 & 0 & 1 & -4 & 1 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 1 & 0 & 0 & 1 & -4 & 1 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 1 & 0 & 0 & 1 & -4 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & -4 & 1 & 0 & 0 & 1 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 1 & -4 & 1 & 0 & 0 & 1 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 1 & -4 & 1 & 0 & 0 & 1 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 1 & -4 & 0 & 0 & 0 & 1 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & -4 & 1 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 1 & -4 & 1 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 1 & -4 & 1 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 1 & -4
\end{bmatrix}
\begin{bmatrix}
T_{2,2} \\ T_{2,3} \\ T_{2,4} \\ T_{2,5} \\ T_{3,2} \\ T_{3,3} \\ T_{3,4} \\ T_{3,5} \\ T_{4,2} \\ T_{4,3} \\ T_{4,4} \\ T_{4,5} \\ T_{5,2} \\ T_{5,3} \\ T_{5,4} \\ T_{5,5}
\end{bmatrix}
=
\begin{bmatrix}
-F_{2,2}\,h^2 \\ -F_{2,3}\,h^2 \\ -F_{2,4}\,h^2 \\ -F_{2,5}\,h^2 \\ -F_{3,2}\,h^2 \\ -F_{3,3}\,h^2 \\ -F_{3,4}\,h^2 \\ -F_{3,5}\,h^2 \\ -F_{4,2}\,h^2 \\ -F_{4,3}\,h^2 \\ -F_{4,4}\,h^2 \\ -F_{4,5}\,h^2 \\ -F_{5,2}\,h^2 - T_0 \\ -F_{5,3}\,h^2 - T_0 \\ -F_{5,4}\,h^2 - T_0 \\ -F_{5,5}\,h^2 - T_0
\end{bmatrix}
\qquad (249)
$$

where $T_{n,m}$ corresponds to the nodal temperatures shown in Figure 22, and $F_{n,m}$ corresponds to the heat generation function at the nodal points (n,m).

81 Interior Nodes

In addition to the 4x4 grid system for the 16 interior nodal points, the finite difference method was used to examine the results when the spacing between adjacent nodes decreased. The original 4x4 grid was subdivided in half, and the temperature at 81 nodes was in a new 9x9 grid network. Instead of generating 81 algebraic equations note that there is a pattern in the diagonal vectors appearing in the

coefficient matrix of expression (249). If the sequential location of the zero elements along any diagonal is known then it is a relative easy manner to generate the entire diagonal vector. Also because there are at most five row elements, from equation (248), in any row of the coefficient matrix only five diagonal vectors have to be stored. A comparison of the two results follow.

Results

The solution of (249) by Gaussian elimination, using the method of finite differences is compared to the exact analytical solution in Table XI. Due to the symmetry in the original problem only half the nodes are tabulated.

Table XI. Finite Difference Solution for Square, with Heat Generation

Node	Exact Solution	Finite Diff 16 Interior	Error	Finite Diff 81 Interior	Error
2,2	4.331240	4.578788	-.247548	4.446669	-.115429
2,3	6.969133	7.243636	-.247503	7.115880	-.146747
3,2	10.555374	11.031515	-.476141	10.755899	-.200525
3,3	16.772428	17.112121	-.339693	16.969429	-.197001
4,2	21.727495	22.395152	-.667657	22.012913	-.285418
4,3	33.090082	33.021212	-.068870	33.166982	-.076900
5,2	45.599465	45.487879	+.111586	45.621920	-.022455
5,3	60.555373	59.516364	+1.039009	60.306397	+.248976

Comment - Finite Differences

The method of finite differences in two-dimensions can be viewed as an averaging process, using the known boundary conditions to generate values at other interior points. The best results are obtained when all nodal points are symmetrical then the boundary values at the edges are 'weighed' more evenly at the interior points. To demonstrate this consider the heat conduction problem as before; the internal temperatures at the point (.5,.5) will be computed by two seperate schemes. The first procedure, shown in Figure 23, is to use three adjacent points located parallel to the x-axis and spaced $h = 1/4$ apart. The temperature, T_1, calculated by the difference equation (248) is

$$T_1 = 23.595588 \tag{250}$$

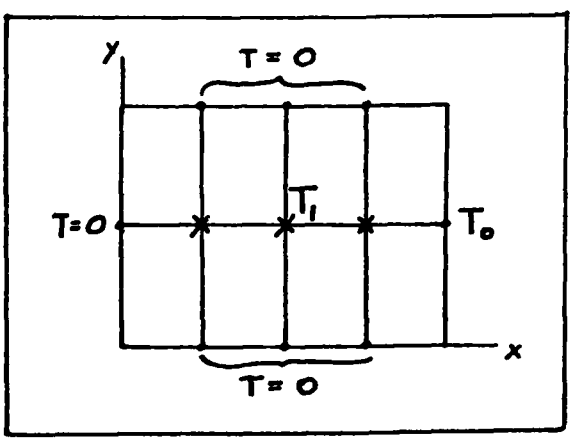

Fig. 23 Finite Difference Scheme Using Three Points Parallel to the X-Axis

The procedure shown in Figure 24, is to use three adjacent points again, but located parallel to the y-axis, spaced $h = 1/4$ apart. T_1 calculated by the difference equation (248) is now found to be

$$T_1 = 26.536765 \tag{251}$$

From the analytical solution, summed over 10,000 separate iterations, the value is 24.926328. The temperature is observed to be greater where the boundary condition T_0 is used three times. It is interesting to note that using only one interior node and equation (248), T_1 is

$$T_1 = 25.0625 \tag{252}$$

This value is only .55% in error from analytical value at (.5,.5).

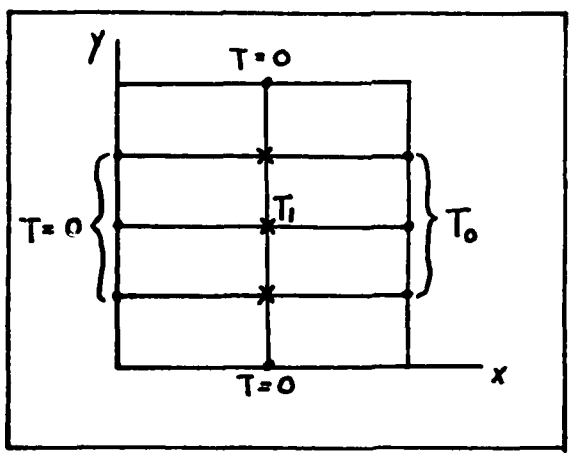

Fig. 24 Finite Difference Scheme Using Three Points Parallel to the y-Axis

Introduction - Splines

The last method to be presented in two-dimensions is the integral solution to the steady-state heat conduction problem using the method of cubic splines.

The integral solution for heat conduction over a rectangular region, with homogeneous Dirichlet boundary conditions, can be expressed in the form

$$T(x,y) = \int_0^a \int_0^b G(x,\xi;y,\eta)\, F(\xi,\eta)\, d\xi\, d\eta \tag{253}$$

where $G(x,\xi;y,\eta)$ is the two-dimensional Green's function for Laplacian (Ref 13: 520-523). If the exact Green's function is known, and $F(\xi,\eta)$ is seperable, equation (253) can be evaluated using the one-dimensional techniques already considered. Many times though, for problems other than rectangular symmetry, the Green's function is extremely difficult to compute; the Green's function depends upon the boundary symmetry, for complicated regions $G(x,\xi;y,\eta)$ can be exceedingly complex. An alternate integral form of solution can be expressed for $T(x,y)$ using splines. The method to be presented was first proposed by Hadjin and Krajcinovic using cubic splines in integral form for solving elliptical partial differential equations (Ref 2: 513-539).

Spline Functions

Because the proposed method uses cubic splines a brief introduction into spline theory is necessary. Spline functions are simply polynominals used to approximate a given function, $f(x)$, over an interval (a,b). However, instead of using a single polynominal over the entire domain the interval (a,b) is divided into subintervals,

$$a = x_1 < x_2 \cdots x_{N-1} < x_N = b \tag{254}$$

with a different polynominal representing $f(x)$ over each subdivision. By definition, a cubic spline is a continuous piecewise function having continuous first and second derivatives everywhere on the interval (a,b) and is represented by a polynominal of degree three or less. Hence, the spline $S_k(x)$ consists of cubic polynominals, one in each of the subintervals (x_{k-1}, x_k).

The cubic spline $S_k(x)$, which approximates $f(x)$ in each interval (x_{k-1}, x_k) can be uniquely determined by insisting that the value of the spline and its first derivatives are equal to the value of $f(x)$ and its first derivatives at each node, x_k:

$$S(x_i) = f(x_i) \quad \text{and} \quad S'(x_i) = f'(x_i) \qquad (i = k-1, k) \tag{255}$$

In addition, to insure a smooth fit of the spline function across the interval (a,b), the values of the

first and second derivatives, on either side of the nodal points x_k will be assumed equal, that is

$$S_k'(x_k-) = S_{k+1}'(x_k+) \tag{256}$$

and

$$S_k''(x_k-) = S_{k+1}''(x_k+) \tag{257}$$

Using the conditions required by expressions (255), (256), and (257), the cubic spline representing $S_k(x)$ can be shown, Appendix E, to be equivalent to

$$S_k(x) = M_{k-1}\frac{(x_k-x)^3}{6h_k} + M_k\frac{(x-x_{k-1})^3}{6h_k}$$

$$+ x\left\{\frac{(y_k-y_{k-1})-(M_k-M_{k-1})(h_k^2/6)}{h_k}\right\} + \left\{\frac{(x_k y_{k-1}-x_{k-1}y_k)-(x_k M_{k-1}-x_{k-1}M_k)(h_k^2/6)}{h_k}\right\} \tag{258}$$

where the symbols are

$$h_k = x_k - x_{k-1}$$
$$M_k = S_k''(x_k)$$
$$y_k = f(x_k)$$

(Ref 14: 296-298)

By using the continuity requirements for the spline, from equation (255), the values of M_k can be determined, namely it is required that

$$\frac{h_k}{6}M_{k-1} + \frac{h_k+h_{k+1}}{3}M_k + \frac{h_{k+1}}{6}M_{k+1}$$

$$= \left\{\frac{1}{h_{k+1}}(y_{k+1}-y_k) - \frac{1}{h_k}(y_k-y_{k-1})\right\} \tag{259}$$

Expression (259) represents a system of N-1 linear algebraic equations with unknowns $M_0, M_1, \ldots, M_N$. By

assigning the values of zero to M_0 and M_N, because the physical sline can be assumed to be straight outside the interval (a,b), i.e., $f''(x) = 0$ for $x < a$ or $x > b$, the other values $M_1, M_2, \ldots, M_{N-1}$ can be determined. Using the spline representation, equation (258), and the continuity requirements, expression (259), the method of splines in the solution of integral equations can now be introduced.

Integral Method of Solution

The steady-state heat conduction problem has the form

$$\frac{\partial^2 T(x,y)}{\partial x^2} + \frac{\partial^2 T(x,y)}{\partial y^2} = -F(x,y) \tag{260}$$

In the method proposed by Hajdin and Krajcinovic the highest derivatives of the function $T(x,y)$ are chosen as the unknown, that is let

$$\frac{\partial^2 T(x,y)}{\partial x^2} = -p(x,y) \quad \text{and} \quad \frac{\partial^2 T(x,y)}{\partial y^2} = -q(x,y) \tag{261}$$

Substituting equations (261) back into equation (260) yields

$$p(x,y) + q(x,y) = F(x,y) \tag{262}$$

Differential equations can now be written for equations (261) for a fixed value of $x = x_k$ and/or $y = y_n$,

$$\frac{d^2 T(x,y_n)}{dx^2} = -p(x,y_n) \quad \text{and} \quad \frac{d^2 T(x_k,y)}{dy^2} = -q(x_k,y) \tag{263}$$

Equations (263) can now be converted into integral form using the Green's function for the differential operators in equations (263). The equivalent integral representation of equations (263) are

$$T(x,y_n) = \int_0^a G(x,\xi)\,p(\xi,y_n)\,d\xi + \frac{T_0 x}{a} \tag{264}$$

and

$$T(x_k,y) = \int_0^b G(y,\eta)\,q(x_k,\eta)\,d\eta \tag{265}$$

where $G(x,\xi)$ and $G(y,\eta)$ are the one-dimensional Green's functions for the second order differential operators appearing in equations (263). Note that the partial differential problem has been converted, along a constant line $x = x_k$ and/or $y = y_n$, into two one-dimensional integral equations. The unknowns $p(\xi,y_n)$ and $q(x_k,\eta)$ are now approximated using cubic splines, given by equation (258) and integrated in equations (264) and (265).

Spline Integration

Using the spline representation, equation (264) becomes

$$T(x_k,y_n) = \left(\frac{a-x_k}{a}\right)\left\{-\frac{x_k^4}{45}M_k + \frac{x_k^2}{3}P_k\right\} + x_k\left\{P_k\frac{(a-x_k)}{2} - \frac{M_k}{24}(a-x_k)^3\right\}$$

$$-\frac{x_k}{a}\left\{\frac{(a-x_k)^4}{45}M_k - \frac{(a-x_k)^3}{24}M_k a - \frac{(a-x_k)^2}{3}P_k + \frac{(a-x_k)}{2}P_k a\right\} + \frac{T_0 x_k}{a} \tag{266}$$

and equation (265) becomes

$$T(x_k, y_n) = \frac{(a-y_n)}{a}\left\{\frac{-y_n^4}{45}N_n + \frac{y_n^2}{3}q_n\right\} + y_n\left\{q_n\frac{(a-y_n)}{2} - \frac{N_n(a-y_n)^3}{24}\right\}$$

$$-\frac{y_n}{}\left\{\frac{(a-y_n)^4}{45}N_n - \frac{(a-y_n)^3}{24}N_n a - \frac{(a-y_n)^2}{3}q_n + \frac{(a-y_n)}{2}q_n a\right\} \qquad (267)$$

where a = length of a side of the square plate

x_k, y_n = location within region

M_k, N_n = value of the second derivative of the spline at (x_k, y_n).

$P_k, q_n = P(x_k, y_n),\ q(x_k, y_n)$

Two expressions for the temperature now exist at the point (x_k, y_n) given by expressions (266) and (267). Because the temperatures must be equivalent at these locations, equations (266) and (267) can be equated. Using the continuity requirements for the second derivatives of the spline functions, given by expression (259), both M_k and N_n can be replaced by a multiple of P_k and q_n. In addition, a second condition exists between P_k and q_n given by equation (262). Therefore, using the two algebraic equations, (266) and (267), and equation (259), the unknowns P_k and q_n can be evaluated. Substituting these values for P_k or q_n back into equations (266) or (267), along with the substituted values of M_k or N_n will yield the temperature at the point (x_k, y_n).

Results

The computed values at the same interior nodes used in the method of finite differences is given in

Table XII. Observe how the error values increase as the node points move away from the center

Table XII. Cubic Spline Solution for Square, with Heat Generation

Node	Exact Solution	Cubic Spline 16 Interior	Error
2,2	4.331240	10.040000	-5.708760
2,4	6.969133	10.617943	-3.648810
3,2	10.555374	18.903657	-8.348283
3,3	16.772428	20.049333	-3.276905
4,2	21.727495	28.332229	-6.604734
4,3	33.090082	30.049333	+3.040749
5,2	45.599465	40.044000	+5.555465
5,3	60.555373	42.332229	+18.223144

Besides the 16 interior points, the grid spacing was halved to observe the effects. Instead of changing the computed values at the node points the exact same values as before were calculated, demonstrating that unlike the finite difference method, the method of cubic splines does not improve by reducing the grid spacing. It is interesting to note that for the most symmetrically located point, (.5,.5), the calculated temperature is within .50% of the actual analytical solution.

Conclusions

The method of finite differences in two-dimensions gives excellent results, the largest relative

error was 5.72% at the node 2,2. Halving the interval spacing resulted in a decrease of this error to 2.67%.

The integral method using cubic splines appears to work well, but only at the most symmetrically located point. The major fault with this method comes when converting the two-dimensional problem into one-dimensional form. Much of the physical significance, the edge effects from the boundaries and the inhomogeneous boundary conditions, have been almost completely neglected. For the particular part of the solution, given by equation (266), no account for the value $y = y_n$ is used though in reality the particular solution is both a function of two variables, x and y. Also there does not appear sufficient coupling to assume that the two seperate splines and condition (262) should result in the same temperature at the point (x_k, y_n); equation (267) is based upon homogeneous boundary conditions and equation (266), for the same point, incorporates two distinctly different boundary conditions. In contrast to what the authors Hajdin and Krajcinovic claim, i.e., that problems of potential theory may be easily and conveniently solved employing the method of cubic splines and integral conversion, the results that were found do not justify, for the reasons cited, the authors claims.

V. Conclusions and Recommendations

Conclusions One-Dimensional Cases

The purpose of this thesis has been to investigate and compare numerical integration techniques with methods based upon numerical differentiation, the finite difference method. In one-dimension the results of this study have been somewhat inconclusive; in the three examples investigated the first two have proven to yield equivalent solutions for both the integral equation approach and the method of central finite differences. This is due to the similarity of the two examples, the Helmholtz equation in Case II was but a modified version of the particular equation for Case I. In addition, the Green's integral approach for Case II was found to yield solutions on the same order of error as the integral and CFD methods. In contrast however, using the particular Cauchy-type equation for Case III, three entirely different results for each method was observed. The Green's integral approach proved to be the most accurate, for only one iteration over the interval (1,3) the computed value was found in error by only .156%. The integral method however for the same equation generated approximately 15 times the error of the Green's integral but for a single iteration the error was still less than 3%. The CFD method had more than

twice the error of the integral method, 6.3%.

Another similarity between Case I and Case II was the fact that both, upon integral conversion, had linear kernels. This can be attributed to the second order differential operator, $\frac{d^2}{dx^2}$, appearing in both differential equations. Case III however, had a non-symmetrical kernel and asymmetric solution, in contrast to the first two cases.

Conclusions Two-Dimensional Cases

The method of finite differences in two-dimensions gives excellent results, at all points, compared to the analytical solution of the steady-state heat conduction problem. In contrast, the integral approach using cubic splines falls short of its expectations at all interior points except the center. The major drawback of the spline technique occurs when the original two-dimensional problem is expressed as two separate one-dimensional cases. The coupling scheme between the splines is no longer valid due to different Dirichlet boundary conditions existing at the plate edges. Another serious drawback to the spline method is that it does not improve as the grid network is decreased. In contrast, the finite difference solutions improve as the grid spacing is reduced.

Recommendations

More study needs be given to a wider variety of one-dimensional problems, using both linear and non-linear kernels. Higher order approximations to the derived difference quotients should also be included to reduce truncation errors in the finite difference technique. In addition, other integration schemes could also be used to see how well specific integral techniques compare to the numerical differentiation techniques. For the two-dimensional analysis a two-dimensional spline function could be tried. The disadvantage of working in two-dimensions though is that the exact form of the Green's function must be known, for complicated geometries this could prove extremely difficult.

In conclusion, there are many areas in which further studies may lead to more fruitful results. This thesis has but presented a brief analysis of several numerical methods for the solution of differential equations in both one and two-dimensions.

Bibliography

1. Hildebrand, F.B. Methods of Applied Mathematics. New York: Prentice-Hall, Inc., 1952.

2. Hajdin, J. and D. Krajcinovic. "Integral Equation Method for the Solution of Boundary Value Problems of Structural Mechanics, Part 2", International Journal for Numerical Methods in Engineering, 4: 523-539 (1972).

3. Hajdin, J. and D. Krajcinovic. "Integral Equation Method for Solution of Boundary Value Problems of Structural Mechanics, Part 1", International Journal for Numerical Methods in Engineering, 4: 509-522 (1972).

4. Irving, J. and N. Mullineus. Mathematics in Physics and Engineering. New York: Academic Press, 1959.

5. Stakgold, Ivar. Boundary Value Problems of Mathematical Physics, Volume I. New York: The Macmillan Company, 1967.

6. Arfken G. Mathematical Methods for Physicists. New York: Academic Press, 1966.

7. Crandall, S.H. Engineering Analysis. New York: McGraw-Hill Book Company, 1956.

8. Salvadori, M.G. Numerical Methods in Engineering. New York: Prentice-Hall, Inc., 1952.

9. Kelly, L.G. Handbook of Numerical Methods and Applications. Reading, Mass.: Addison-Wesley Publishing Company, 1967.

10. Hornbeck, R.W. Numerical Methods. New York: Quantum Publishers, Inc., 1975.

11. Forsythe, G. and C.B. Moler. Computer Solutions of Linear Algebraic Systems. Englewood Cliffs, N.J.: Prentice-Hall Inc., 1967.

12. Flanders, H., R.R. Korthage, and J.J. Price. Calculus. New York: Academic Press, 1970.

13. Butkov, E. Mathematical Physics. Reading, Mass.: Addison-Wesley Publishing Company, 1968.

14. Young, D.M. and R.T. Gregory. A Survey of Numerical Mathematics, Volume I. Reading, Mass.: Addison-Wesley Publishing Company, 1973.

15. Gallof, S. A Numerical Investigation and Utilization of Green's Functions. Unpublished Thesis. Wright-Patterson Air Force Base, Ohio: Air Force Institute of Technology, June 1968.

Appendix A

Kernel Properties of the Equation $\frac{d^2y}{dx^2} + A\frac{dy}{dx} + By = 0$ for $A \neq 0$.

A differential equation of the form

$$\frac{d^2y}{dx^2} + A\frac{dy}{dx} + By = 0 \tag{268}$$

with homogeneous Dirichlet boundary conditions

$$y(0) = 0, \qquad y(\ell) = 0 \tag{269}$$

will have a non-symmetrical kernel when expressed in integral form if $A \neq 0$. In order to demonstrate this, rewrite equation (268) in the form

$$\frac{d^2y}{dx^2} = -A\frac{dy}{dx} - By \tag{270}$$

and integrate both sides over the interval $(0, x)$. Equation (270) now becomes

$$\left.\frac{dy}{dx}\right|_0^x = -A\int_0^x \frac{dy}{dx}\,dx - B\int_0^x y\,dx \tag{271}$$

or

$$\frac{dy(x)}{dx} - \frac{dy(0)}{dx} = -A\,y(x) - B\int_0^x y\,dx \tag{272}$$

Let C donote the constant $\frac{dy(0)}{dx}$ and integrate equation (272) a second time over the same limits as before. Expression (272) becomes

$$\int_0^x \frac{dy}{dx}\,dx = C\int_0^x dx - A\int_0^x y(x)\,dx - B\int_0^x\int_0^x y\,dx\,dx \tag{273}$$

Now, using the results of equation (6) and changing the dummy variable of integration in the second integral on the right-hand side of equation (273) it is found that

$$y(x) = Cx - A\int_0^x y(\xi)d\xi - B\int_0^x (x-\xi)\,y(\xi)d\xi \tag{274}$$

Applying the boundary conditions at $y(\ell)$ evaluates the constant C, that is

$$y(\ell) = 0 = C\ell - A\int_0^\ell y(\xi)d\xi - B\int_0^\ell (\ell-\xi)\,y(\xi)d\xi \tag{275}$$

$$\therefore \quad C = \frac{1}{\ell}\int_0^\ell \left\{A + B(\ell-\xi)\right\} y(\xi)\,d\xi \tag{276}$$

and equation (274), using C above becomes

$$y(x) = \frac{x}{\ell}\int_0^\ell \left\{A + B(\ell-\xi)\right\} y(\xi)\,d\xi - \int_0^x \left\{A + B(x-\xi)\right\} y(\xi)\,d\xi \tag{277}$$

Expressing the first integral as $\int_0^\ell = \int_0^x + \int_x^\ell$ becomes

$$y(x) = \int_0^x \left\{\frac{x-1}{\ell}\right\}(A - B\xi)\,y(\xi)d\xi + \int_x^\ell \frac{x}{\ell}\left(A + B(\ell-\xi)\right)y(\xi)d\xi \tag{278}$$

The kernel in the above integral equation expression can be identified by making the substitution

$$y(x) = \int_0^\ell K(x,\xi)\,y(\xi)\,d\xi \tag{279}$$

where the abbreviation for the kernel is

$$K(x,\xi) = \begin{cases} \dfrac{Ax}{\ell} + \dfrac{Bx}{\ell}(\ell-\xi) \\[2ex] \dfrac{A(x-1)}{\ell} - B\xi\left(\dfrac{x}{\ell} - 1\right) \end{cases} \tag{280}$$

Note that the kernel is both non-symmetric and discontinuous at $x = \xi$, unless $A = 0$.

Appendix B

Determining the Green's Function for the One-Dimensional Helmholtz Equation

The differential equation for the one-dimensional Helmholtz equation is

$$\frac{d^2y}{dx^2} + \lambda^2 y = -f(x) \tag{281}$$

The Green's function for the differential operator, i.e., the left side of expression (281), must satisfy the following differential equation

$$\frac{d^2G(x,\xi)}{dx^2} + \lambda^2 G(x,\xi) = -\delta(x-\xi) \tag{282}$$

Because $G(x,\xi)$ can be thought of as a function of only one variable for a constant ξ, assume that the Green's function can be expressed by $G_1(x)$ and $G_2(x)$ over some interval $(0,\ell)$. The Green's function will be of the form

$$G(x,\xi) = \begin{cases} G_1(x) & x < \xi \\ G_2(x) & x > \xi \end{cases} \tag{283}$$

for $x \neq \xi$ $G_1(x)$ and $G_2(x)$ will each satisfy the homogeneous equation of expression (282), that is

$$\frac{d^2G_1(x)}{dx^2} + \lambda^2 G_1(x) = 0 \tag{284}$$

and

$$\frac{d^2G_2(x)}{dx^2} + \lambda^2 G_2(x) = 0 \tag{285}$$

The solution of the homogeneous equations (284) and (285)

yield, for $G_1(x)$ and $G_2(x)$, the Green's function

$$G(x,\xi) = \begin{cases} A\cos\lambda x + B\sin\lambda x & x<\xi \\ D\cos\lambda x + E\sin\lambda x & x>\xi \end{cases} \tag{286}$$

The Green's function has the property of being zero at the end points and therefore two of the constants in expression (286) can be evaluated. Using the boundary values for $G(x,\xi)$ at the end points it is found that

$$G_1(0) = 0 = A \tag{287}$$

$$G_2(\ell) = 0 = D\cos\lambda\ell + E\sin\lambda\ell \tag{288}$$

Substituting the above values back into equation (286) $G(x,\xi)$ becomes

$$G(x,\xi) = \begin{cases} B\sin\lambda x & x<\xi \\ D\cos\lambda x - D\dfrac{\cos\lambda\ell}{\sin\lambda\ell}\sin\lambda x & x>\xi \end{cases} \tag{289}$$

Because the Green's function is continuous across the entire interval $G_1(\xi) = G_2(\xi)$. Using this condition in equation (289) above will further reduce the unknown constants

$$B\sin\lambda\xi = D\cos\lambda\xi - D\frac{\cos\lambda\ell}{\sin\lambda\ell}\sin\lambda\xi \tag{290}$$

$$\therefore \quad B = D\frac{\cos\lambda\xi}{\sin\lambda\xi} - D\frac{\cos\lambda\ell}{\sin\lambda\ell} \tag{291}$$

and expression (289) becomes

$$G(x,\xi) = \begin{cases} D\left\{\dfrac{\cos\lambda\xi}{\sin\lambda\xi} - \dfrac{\cos\lambda l}{\sin\lambda l}\right\}\sin\lambda x & x<\xi \\ D\left\{\cos\lambda x - \dfrac{\cos\lambda l}{\sin\lambda l}\sin\lambda x\right\} & x>\xi \end{cases} \tag{292}$$

The last property of the Green's function is that at the discontinuity $x=\xi$, the derivative of $G(x,\xi)$ has the magnitude $-1/p(\xi)$ or -1 by expressing equation (282) in self-adjoint form. The discontinuity becomes

$$\frac{dG_2(x)}{dx} - \frac{dG_1(x)}{dx} = -1 \tag{293}$$

Using the terms of expression (292) and substituting into equation (293) the constant D is found to be

$$D = \frac{\sin\lambda\xi}{\lambda} \tag{294}$$

This value of D can now be substituted back into equation (292) and after several algebraic manipulations becomes

$$G(x,\xi) = \begin{cases} \dfrac{\sin\lambda x}{\lambda\sin\lambda l}\sin\lambda(l-\xi) & x<\xi \\ \dfrac{\sin\lambda\xi}{\lambda\sin\lambda l}\sin\lambda(l-x) & x>\xi \end{cases} \tag{295}$$

Appendix C

Determining the Green's Function for Case III

The differential equation for the one-dimensional Cauchy-type equation is

$$x^2 \frac{d^2y}{dx^2} - 2y = x^4 \tag{296}$$

In order to determine the Green's function for a differential operator the operator must first be expressed in self-adjoint form, that is, it must appear as

$$\frac{d}{dx}\left(p(x)\frac{d}{dx}\right) + q(x) \tag{297}$$

Equation (296) is not expressed in self-adjoint form but can be by dividing through by x^2. The Green's function must satisfy the differential equation

$$\frac{d^2G(x,\xi)}{dx^2} - \frac{2}{x^2}G(x,\xi) = -\delta(x-\xi) \tag{298}$$

Because $G(x,\xi)$ can be considered as two separate functions, $G_1(x)$ and $G_2(x)$, the Green's function will be of the form

$$G(x,\xi) = \begin{cases} G_1(x) & x < \xi \\ G_2(x) & x > \xi \end{cases} \tag{299}$$

For $x \neq \xi$ $G_1(x)$ and $G_2(x)$ will each satisfy the homogeneous equation of expression (298), that is

$$\frac{d^2G_1(x)}{dx^2} - \frac{2}{x^2}\,G_1(x) = 0 \tag{300}$$

and

$$\frac{d^2G_2(x)}{dx^2} - \frac{2}{x^2}\,G_2(x) = 0 \tag{301}$$

The solution of equations (300) and (301) can be obtained by substituting

$$G = x^m \tag{302}$$

from which $m = -1, 2$ can be found. Therefore the Green's function takes the form

$$G(x,\xi) = \begin{cases} Ax^{-1} + Bx^2 & x < \xi \\ Cx^{-1} + Dx^2 & x > \xi \end{cases} \tag{303}$$

Utilizing the fact that $G(x,\xi)$ is always zero at the end points over the interval (1,3) two of the constants in expression (303) can be evaluated, it is found that

$$G_1(1) = 0 = A + B \quad \therefore \quad B = -A \tag{304}$$

$$G_2(3) = 0 = \frac{C}{3} + 9D \quad \therefore \quad D = -\frac{C}{27} \tag{305}$$

Substituting the values for B and D into equation (303) the Green's function becomes

$$G(x,\xi) = \begin{cases} A\left(\frac{1}{x} - x^2\right) & x < \xi \\ C\left(\frac{1}{x} - \frac{x^2}{27}\right) & x > \xi \end{cases} \tag{306}$$

Next, using the continuity property of the Green's function, namely

$$G_1(\xi) = G_2(\xi) \tag{307}$$

it is found that

$$A\left(\xi^{-1} - \xi^2\right) = C\left(\xi^{-1} - \frac{\xi^2}{27}\right) \tag{308}$$

$$\therefore\ A = C\left(\xi^{-1} - \frac{\xi^2}{27}\right) \Big/ \left(\xi^{-1} - \xi^2\right) \tag{309}$$

Substituting expression (309) back into equation (306) for $G_1(x)$ will give

$$G(x,\xi) = \begin{cases} \left\{C\left(\xi^{-1} - \frac{\xi^2}{27}\right) \Big/ \left(\xi^{-1} - \xi^2\right)\right\}\left(x^{-1} - x^2\right) & x < \xi \\ C\left(x^{-1} - \frac{x^2}{27}\right) & x > \xi \end{cases} \tag{310}$$

The constant C can be evaluated by using the discontinuity property in the first derivative of the Green's function, i.e.,

$$\frac{dG_2(\xi)}{dx} - \frac{dG_1(\xi)}{dx} = -1 \tag{311}$$

Differentiating both terms in expression (310) and substituting into equation (311) gives

$$C = \frac{27}{78}\left(\xi^2 - \frac{1}{\xi}\right) \tag{312}$$

The value of C can now be substituted back into expression (310) for the Green's function, which after simplifying becomes

$$G(x,\xi) = \begin{cases} \frac{27}{78}\left(\frac{\xi^2}{27} - \frac{1}{\xi}\right)\left(x^{-1} - x^2\right) & x < \xi \\ \frac{27}{78}\left(\xi^2 - \frac{1}{\xi}\right)\left(x^{-1} - \frac{x^2}{27}\right) & x > \xi \end{cases} \tag{313}$$

Appendix D

Analytic Solution for the Two-Dimensional Steady-State Heat Conduction Problem

The two-dimensional Poisson equation representing the internal temperature within some enclosed region is given explicitly by the partial differential equation

$$\nabla^2 T^*(x,y) = -F(x,y) \tag{314}$$

where $T^*(x,y)$ is the temperature at the point (x,y) and $F(x,y)$ represents the internal heat generation from some source. The solution of equation (314) will be derived over a square plate with the Dirichlet boundary values

$$T(x,0) = T(0,y) = T(x,b) = 0, \qquad T(a,y) = T_0 \tag{315}$$

where T_0 is a constant temperature along the edge $X = a$.

Applying the superposition principle the problem can be simplified by assuming that the complete solution for $T^*(x,y)$ can be represented by two independent harmonic functions. The first of these satisfies equation (314) but with homogeneous Dirichlet boundary conditions. The second harmonic function satisfies the Laplacian of (314) using the inhomogeneous boundary condition at $X = a$. The complete solution is then given by the superposition of both harmonic functions, see Figure 25, that is

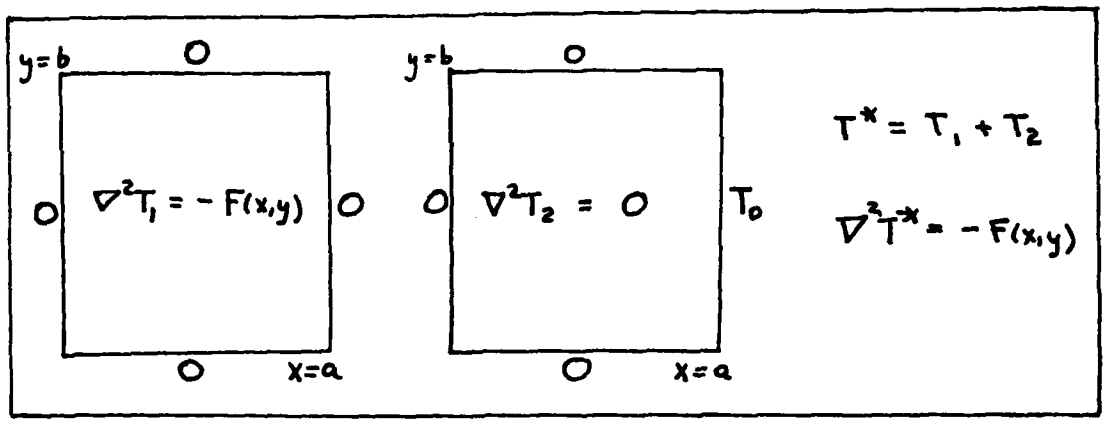

Fig. 25 Method of Harmonic Solutions for the Poisson Equation

$$T^* = T_1 + T_2 \tag{316}$$

or

$$\nabla^2 T^* = -F(x,y) \tag{317}$$

and therefore T^* satisfies the original Poisson equation but is composed of the two harmonic functions T_1 and T_2 .

Poisson's equation, with the homogeneous boundary conditions, can be solved by assuming that $F(x,y)$ can be represented as an eign-function of T_1 , that is

$$-F(x,y) = \lambda T_1 \tag{318}$$

Substituting this value for $F(x,y)$ will give the partial differential equation

$$\frac{\partial^2 T_1}{\partial x^2} + \frac{\partial^2 T_1}{\partial y^2} = \lambda T_1 \tag{319}$$

By using the method of separation of variables for T_1 , i.e., $T_1 = X \cdot Y$, the two eign-functions are obtained

$$X(x) = A \sin \frac{n\pi x}{a} \quad \text{and} \quad Y(y) = B \sin \frac{m\pi y}{b} \tag{320}$$

with

$$\lambda = \left(\frac{n^2\pi^2}{a^2} + \frac{m^2\pi^2}{b^2} \right) \tag{321}$$

Therefore T_1 it is found

$$T_1 = A_{nm} \sin \frac{n\pi x}{a} \sin \frac{m\pi y}{b} \tag{322}$$

Because of linear superposition an infinite series of equation (322) will also satisfy the original differential equation, therefore T_1 is of the form

$$T_1 = \sum_n \sum_m A_{nm} \sin \frac{n\pi x}{a} \sin \frac{m\pi y}{b} \tag{323}$$

Substituting expression (323) for T_1 into equation (318) the following expression results

$$-F(x,y) = \lambda \sum_n \sum_m A_{nm} \sin \frac{n\pi x}{a} \sin \frac{m\pi y}{b} \tag{324}$$

Solving for the coefficient A_{nm} it is found that

$$A_{nm} = -\frac{4}{ab\lambda} \int_0^a \int_0^b F(x,y) \sin \frac{n\pi x}{a} \sin \frac{m\pi y}{b} \, dx\, dy \tag{325}$$

For $F(x,y) = 1$, the coefficient becomes

$$A_{nm} = \frac{-16a^2b^2}{nm\pi^4(a^2m^2 + b^2n^2)} \tag{326}$$

and T_1, from expression (323), becomes

$$T_1 = -\sum_n \sum_m \frac{16a^2b^2}{nm\pi^4(a^2m^2+b^2n^2)} \sin\frac{n\pi}{a}x \sin\frac{m\pi}{b}y \tag{327}$$

The second harmonic function, T_2, satisfies the Laplacian of equation (314) and has the inhomogeneous boundary condition of T_0 at $x=a$. The Laplacian of T_2 is

$$\nabla^2 T_2 = \frac{\partial^2 T_2}{\partial x^2} + \frac{\partial^2 T_2}{\partial y^2} = 0 \tag{328}$$

Again, using the method of separation of variables for T_2, the two eignfunctions are obtained

$$X(x) = A \sinh\frac{n\pi}{b}x \quad \text{and} \quad Y(y) = B \sin\frac{n\pi}{b}y \tag{329}$$

Therefore T_2 becomes

$$T_2 = X \cdot Y = B_n \sinh\frac{n\pi}{b}x \sin\frac{n\pi}{b}y \tag{330}$$

Using the linear superposition principle equation (330) becomes

$$T_2 = \sum_n B_n \sinh\frac{n\pi}{b}x \sin\frac{n\pi}{b}y \tag{331}$$

The inhomogeneous boundary condition at $x=a$ can now be applied to evaluate B_n, that is

$$T_2(a,y) = T_0 = \sum_n B_n \sinh\frac{n\pi a}{b} \sin\frac{n\pi}{b}y \tag{332}$$

and B_n is found to be

$$B_n = \frac{4T_0}{n\pi \sinh \frac{n\pi a}{b}} \tag{333}$$

Substituting this value for B_n into equation (331), T_2 is found to be

$$T_2 = \sum_n \frac{4T_0}{n\pi} \frac{\sinh \frac{n\pi x}{b}}{\sinh \frac{n\pi a}{b}} \cdot \sin \frac{n\pi y}{b} \tag{334}$$

The complete solution for T^* is now given by equations (327) and (334)

$$T^* = T_1 + T_2 = -\frac{16a^2b^2}{\pi^4} \sum_n \sum_m \frac{\sin \frac{n\pi x}{a} \sin \frac{m\pi y}{b}}{nm(a^2m^2 + b^2n^2)}$$

$$+ \frac{4T_0}{\pi} \sum_n \frac{\sinh \frac{n\pi x}{b}}{n \cdot \sinh \frac{n\pi a}{b}} \cdot \sin \frac{n\pi y}{b} \tag{335}$$

Appendix E

Derivation of the Cubic Spline Function

The spline function, $S_k(x)$, is a polynominal of degree three or less on the subinterval

$$I_k = [\, x_{k-1}, x_k \,] \tag{336}$$

and will satisfy the conditions that

$$S(x_i) = f(x_i), \quad \text{and} \quad S'(x_i) = f'(x_i) \qquad (i = k-1, k) \tag{337}$$

Equation (337) imposes the conditions that the spline function have the same values as $f(x)$ and its first derivative at each node location. This will allow $S(x)$ to be substituted for $f(x)$ on each interval, I_k . To insure a smooth fit of adjacent splines across the entire interval (a, b) it will be required that

$$S_k'(x_k-) = S_{k+1}'(x_k+) \tag{338}$$

and

$$S_k''(x_k-) = S_{k+1}''(x_k+) \tag{339}$$

Expressions (338) and (339) assure a smoth fit of adjoining splines at each interior node, x_k . Since $S_k(x)$ is a cubic polynominal, $S_k''(x)$ is a linear function of x on the interval I_k . The second derivative of the spline will appear as

$$S_k''(x) = M_{k-1}\frac{(x_k - x)}{(x_k - x_{k-1})} + M_k\frac{(x - x_{k-1})}{(x_k - x_{k-1})} \tag{340}$$

where

$$M_k = S_k''(x_k) \tag{341}$$

Expression (340) can be obtained, from Figure 26, by solving for $M_k(x)$ using the linear slope, $\frac{M_k - M_{k-1}}{x_k - x_{k-1}}$, across the interval (x_{k-1}, x_k).

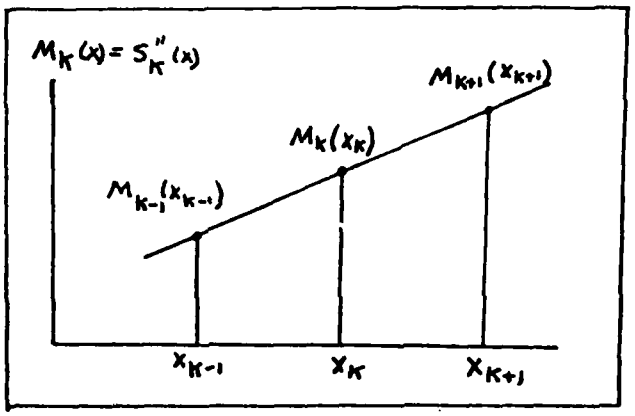

Fig. 26 Derivative of Cubic Spline Function, $S_k(x)$

Integrate equation (340) to find:

$$S_k'(x) = -\frac{M_{k-1}(x_k - x)^2}{2h_k} + \frac{M_k(x - x_{k-1})^2}{2h_k} + C_1 \tag{342}$$

where C_1 is a constant from the integration and $h_k = x_k - x_{k-1}$. Integrating again, the spline function is found:

$$S_k(x) = \frac{M_{k-1}(x_k - x)^3}{6h_k} + \frac{M_k(x - x_{k-1})^3}{6h_k} + C_1 x + C_2 \tag{343}$$

Let $y_K = f(x_k)$, and using condition (337), $y_K = S_K(x_k)$. Therefore

$$y_{k-1} = S_{K-1}(x_{k-1}) = \frac{M_{k-1} h_k^2}{6} + c_1 x_{k-1} + c_2 \tag{344}$$

and

$$y_K = S_K(x_k) = \frac{M_K h_k^2}{6} + c_1 x_K + c_2 \tag{345}$$

Solving for c_1 and c_2 :

$$c_1 = \frac{(y_K - y_{K-1}) - (M_K - M_{K-1})(h_k^2/6)}{h_K} \tag{346}$$

and

$$c_2 = \frac{(x_K y_{k-1} - x_{k-1} y_k) - (x_K M_{k-1} - x_{k-1} M_k)(h_k^2/6)}{6} \tag{347}$$

Substituting expressions (346) and (347) back into equation (343) the cubic spline becomes

$$S_k(x) = \frac{M_{k-1}(x_k - x)^3}{6 h_K} + \frac{M_k (x - x_{k-1})^3}{6 h_K}$$

$$+ \left\{ \frac{(y_k - y_{k-1}) - (M_K - M_{k-1})(h_k^2/6)}{h_K} \right\} x$$

$$+ \left\{ \frac{(x_K y_{k-1} - x_{k-1} y_k) - (x_K M_{k-1} - x_{k-1} M_K)(h_k^2/6)}{h_K} \right\} \tag{348}$$

Appendix F

Integration, Using the Cubic Spline Function

The integral representation for the temperature along the line $y = y_n$ is given by equation (264) as

$$T(x, y_n) = \int_0^a G(x,\xi)\, p(\xi, y_n)\, d\xi + \frac{T_0 x}{a} \tag{349}$$

The one-dimensional Green's function, $G(x,\xi)$ is given by the expression

$$G(x,\xi) = \begin{cases} \dfrac{x(a-\xi)}{a} & x < \xi \\ \dfrac{\xi(a-x)}{a} & x > \xi \end{cases} \tag{350}$$

Substituting in $G(x,\xi)$, over the appropriate limits, (349) becomes

$$T(x, y_n) = \int_0^x \frac{\xi(a-x)}{a}\, p(\xi, y_n)\, d\xi + \int_x^a \frac{x(a-\xi)}{a}\, p(\xi, y_n)\, d\xi + \frac{T_0 x}{a} \tag{351}$$

The value of the temperature at the node x_K is found by substituting $x = x_K$ into (351) above and is expressed as

$$T(x_K, y_n) = \int_0^{x_K} \frac{\xi(a-x_K)}{a}\, p(\xi, y_n)\, d\xi + \int_{x_K}^a \frac{x_K(a-\xi)}{a}\, p(\xi, y_n)\, d\xi + \frac{T_0 x_K}{a} \tag{352}$$

Since a and x_k are constant, and because $p(\xi, y_n)$ is only a function of the variable ξ for constant y_n, equation (352) simplifies to

$$T(x_k, y_n) = \left(\frac{a - x_k}{a}\right) \int_0^{x_k} \xi\, p(\xi)\, d\xi + x_k \int_{x_k}^{a} p(\xi)\, d\xi$$

$$- \frac{x_k}{a} \int_{x_k}^{a} \xi\, p(\xi)\, d\xi + \frac{T_0 x_k}{a} \tag{353}$$

Now, $p(\xi)$ will approximated by the cubic spline representation given by equation (258), substituted back into the integral, equation (353), and integrated. The results after much algebraic manipulation yield

$$\int_0^{x_k} \xi\, p(\xi)\, d\xi = -\frac{x_k^4}{45} M_k + \frac{x_k^2}{3} P_k \tag{354}$$

$$\int_{x_k}^{a} \xi\, p(\xi)\, d\xi = \frac{P_k}{2}(a - x_k) - \frac{M_k}{24}(a - x_k)^3 \tag{355}$$

$$\int_{x_k}^{a} p(\xi)\, d\xi = \frac{(a-x_k)^4}{45} M_k - \frac{(a-x_k)^3}{24} M_k a - \frac{(a-x_k)^2}{3} P_k + \frac{(a-x_k)}{2} P_k a \tag{356}$$

Replacing the integrals, given in equation (353) by their equivalent quantities above, equation (353) becomes

$$T(x_k, y_n) = \left(\frac{a - x_k}{a}\right)\left\{ -\frac{x_k^4 M_k}{45} + \frac{x_k^2 P_k}{3} \right\}$$

$$+ \; x_k \left\{ P_k \left(\frac{a - x_k}{2}\right) - \frac{M_k}{24}(a - x_k)^3 \right\}$$

$$- \frac{x_k}{a}\left\{ \frac{(a - x_k)^4}{45} M_k - \frac{(a - x_k)^3}{24} M_k a - \frac{(a - x_k)^2}{3} P_k + \frac{(a - x_k)}{2} P_k a \right\}$$

$$+ \; \frac{T_0 x_k}{a} \qquad (357)$$

Vita

Gale N. Nelson was born on 24 March 1950 in Lawrence, Kansas, the son of Albert V. Nelson and Dorthy M. Nelson. After graduating from Mar Vista High School in Imperial Beach, California in 1968, he enrolled at Southwestern Junior College and received an A.S. degree in June 1970. In September of 1970 he transferred to San Diego State University and received the degree of Bachelor of Science in Physics in June 1973. He attended Undergraduate Navigator Training School at Mather AFB, California and graduated as an Outstanding Graduate in July 1973. Assigned to the 4th Military Airlift Squadron at McChord AFB, Washington in October 1973, he participated in frequent airlift missions to the Far East and Europe. Upgrading to instructor navigator in December 1976 he has accumulated over 2,000 flying hours in the C-141 aircraft. He was assigned to the Air Force Institute of Technology in June 1978.

Permanent address: 708 Oneonta Ave.
Imperial Beach, California
92032

Unclassified

SECURITY CLASSIFICATION OF THIS PAGE (When Data Entered)

REPORT DOCUMENTATION PAGE		READ INSTRUCTIONS BEFORE COMPLETING FORM
1. REPORT NUMBER AFIT/GEP/PH/79D-7	2. GOVT ACCESSION NO.	3. RECIPIENT'S CATALOG NUMBER
4. TITLE (and Subtitle) NUMERICAL METHODS AND THE SOLUTION OF BOUNDARY VALUE PROBLEMS		5. TYPE OF REPORT & PERIOD COVERED MS Thesis 6. PERFORMING ORG. REPORT NUMBER
7. AUTHOR(s) Gale N. Nelson Captain, USAF		8. CONTRACT OR GRANT NUMBER(s)
9. PERFORMING ORGANIZATION NAME AND ADDRESS Air Force Institute of Technology (AFIT-EN) Wright-Patterson AFB, Ohio 45433		10. PROGRAM ELEMENT, PROJECT, TASK AREA & WORK UNIT NUMBERS
11. CONTROLLING OFFICE NAME AND ADDRESS Air Force Materials Laboratory (AML/MBC) Wright-Patterson AFB, Ohio 45433		12. REPORT DATE December, 1979 13. NUMBER OF PAGES 142
14. MONITORING AGENCY NAME & ADDRESS(if different from Controlling Office)		15. SECURITY CLASS. (of this report) Unclassified 15a. DECLASSIFICATION/DOWNGRADING SCHEDULE

16. DISTRIBUTION STATEMENT (of this Report)

Approved for public release; distribution unlimited

17. DISTRIBUTION STATEMENT (of the abstract entered in Block 20, if different from Report)

18. SUPPLEMENTARY NOTES

Approved for public release; IAW AFR 190-17

JOSEPH P. HIPPS, Maj, USAF
Director of Public Affairs

19. KEY WORDS (Continue on reverse side if necessary and identify by block number)

Green's Functions
Numerical Methods
Integral Equations
Finite Differences
Boundary Value Problems
Cubic Splines

20. ABSTRACT (Continue on reverse side if necessary and identify by block number)

A study of several numerical methods for the solution of boundary value problems, in both one and two-dimensions, was conducted using the CDC 6600 computer. The method of finite differences was employed for solution of the equations in differential form. These numerical solutions were compared to those obtained by transforming the original differential equation into integral form and approximating their solution using numerical integration via trapezoid rule. All numerical experiments were conducted using

DD FORM 1 JAN 73 1473 EDITION OF 1 NOV 65 IS OBSOLETE

Unclassified

SECURITY CLASSIFICATION OF THIS PAGE (When Data Entered)

20. Dirichlet boundary conditions.

In the one-dimensional cases studied it was found that both methods are equivalent, i.e., yield identical solutions when the integral representation had a linear weighted Green's function kernel. The integral approach was found to be as accurate in all one-dimensional cases as the method of finite differences.

For the two-dimensional investigation the steady-state heat conduction equation was analyzed. The method of finite differences was compared to the integral approach, using cubic splines. The method of finite differences was found to be superior in calculating the internal temperature, at all nodal points, as compared to the integral-spline solution.